



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:39 PM UTC

PDB ID : 5NDF / pdb_00005ndf
Title : Small-molecule inhibition of ppGalNAc-Ts selectively reduces mucin-type O-glycosylation
Authors : Hurtado-Guerrero, R.; De las Rivas, M.
Deposited on : 2017-03-08
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

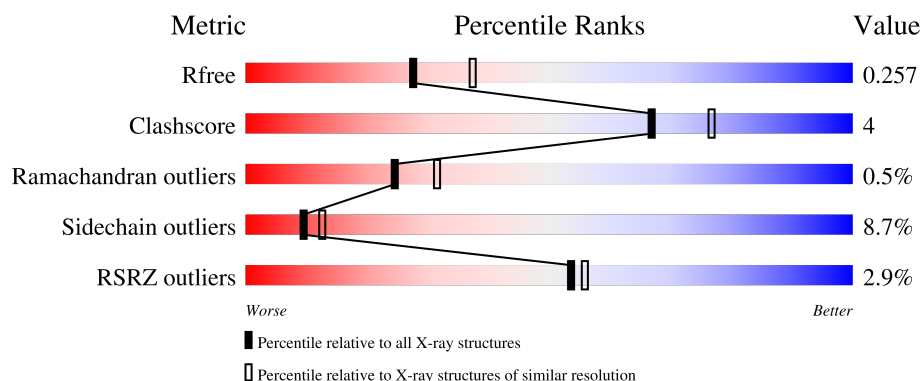
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	571	74% 10% • 13%
1	B	571	74% 10% • 13%
1	C	571	74% 9% •• 13%
1	D	571	75% 9% • 13%
1	E	571	74% 10% • 14%

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Mol	Chain	Length	Quality of chain
1	F	571	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	LU2	A	608	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24971 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Polypeptide N-acetylgalactosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	20	2	0
			3976	2503	720	729	24			
1	B	495	Total	C	N	O	S	20	2	0
			3983	2507	725	727	24			
1	C	495	Total	C	N	O	S	20	3	0
			3987	2510	724	729	24			
1	D	495	Total	C	N	O	S	20	2	0
			3983	2507	725	727	24			
1	E	492	Total	C	N	O	S	20	3	0
			3962	2493	719	726	24			
1	F	495	Total	C	N	O	S	20	1	0
			3973	2501	720	728	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ASP	ASN	engineered mutation	UNP Q10471
B	516	ASP	ASN	engineered mutation	UNP Q10471
C	516	ASP	ASN	engineered mutation	UNP Q10471
D	516	ASP	ASN	engineered mutation	UNP Q10471
E	516	ASP	ASN	engineered mutation	UNP Q10471
F	516	ASP	ASN	engineered mutation	UNP Q10471

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

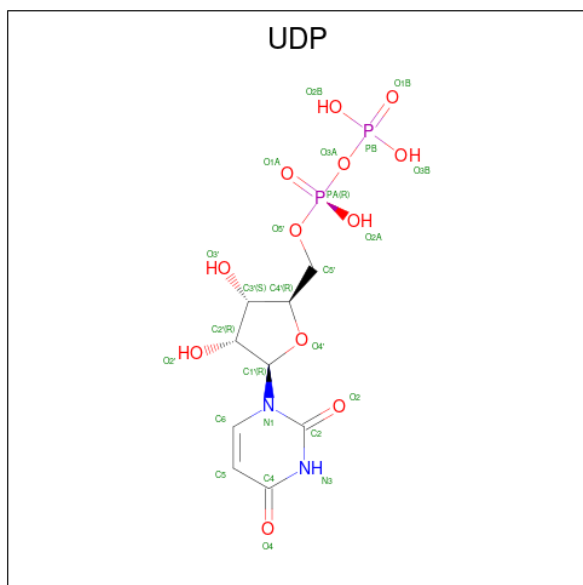
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

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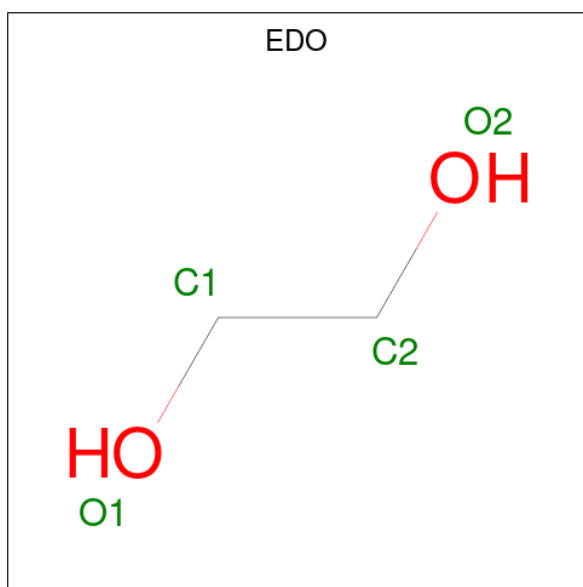
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



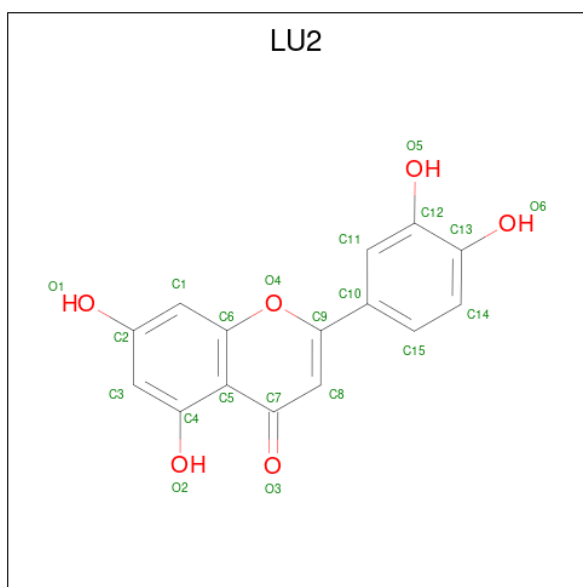
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-chromen-4-one (CCD ID: LU2) (formula: C₁₅H₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			21	15	6		
5	B	1	Total	C	O	0	0
			21	15	6		
5	D	1	Total	C	O	0	0
			21	15	6		

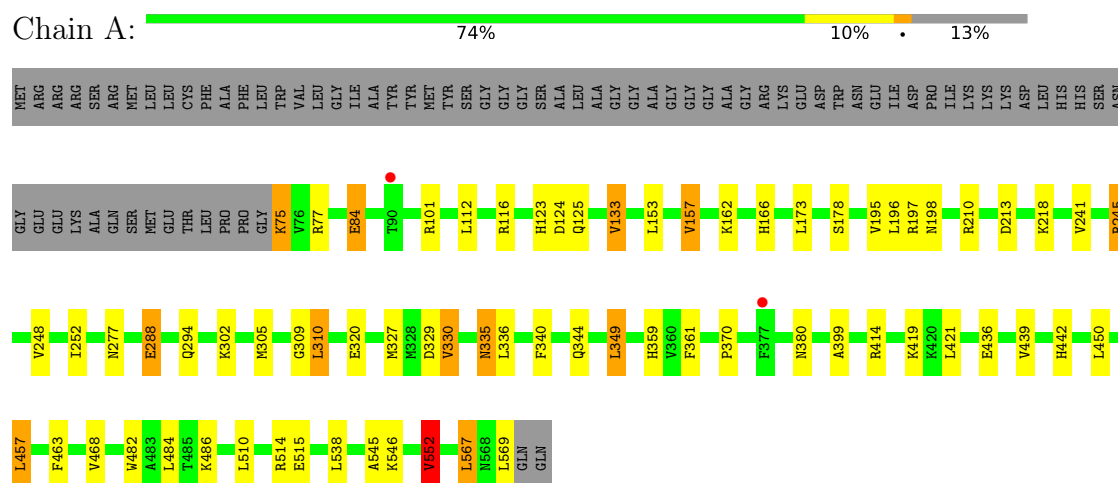
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	194	Total	O	0	0
			194	194		
6	B	147	Total	O	0	0
			147	147		
6	C	138	Total	O	0	0
			138	138		
6	D	163	Total	O	0	0
			163	163		
6	E	117	Total	O	0	0
			117	117		
6	F	89	Total	O	0	0
			89	89		

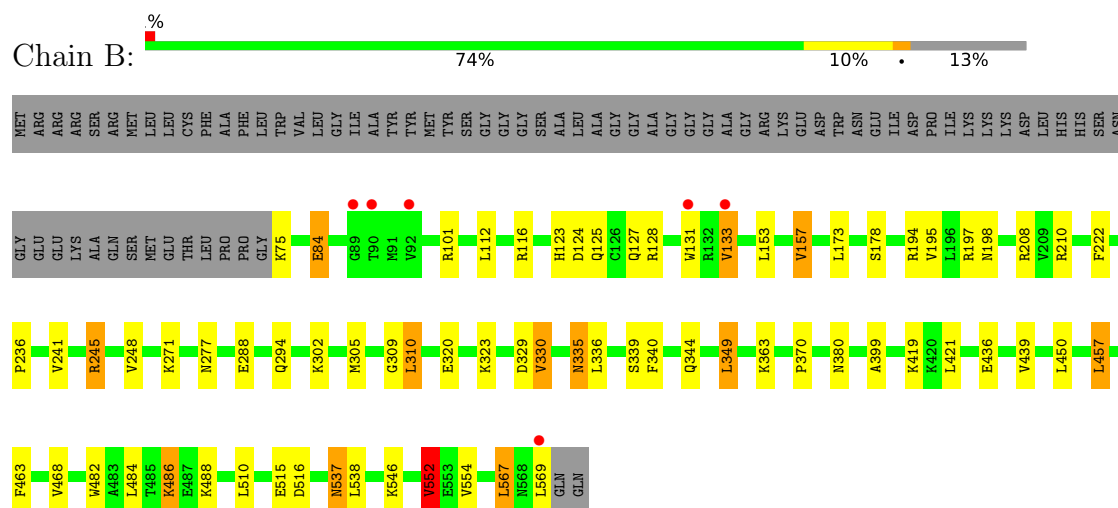
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

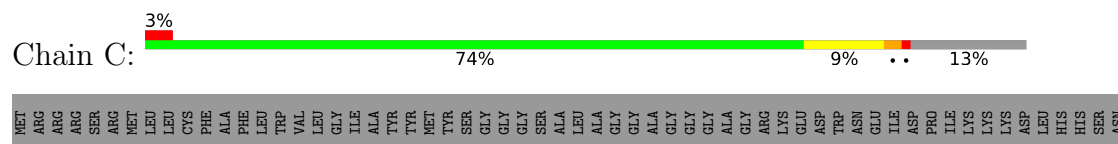
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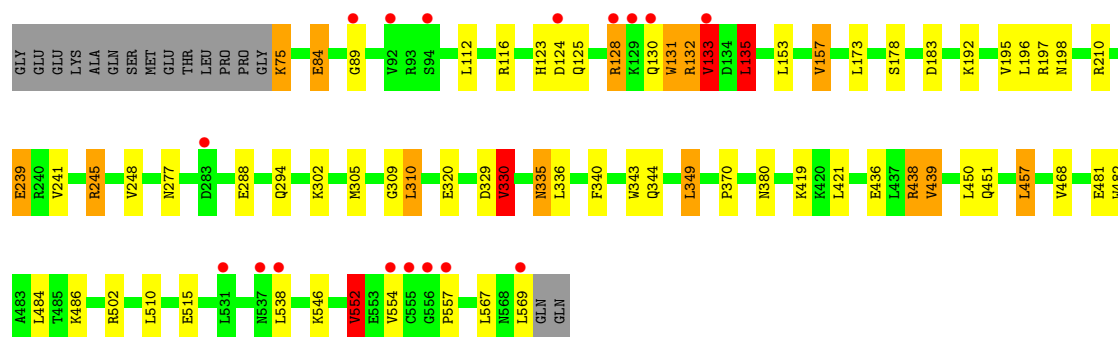


• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

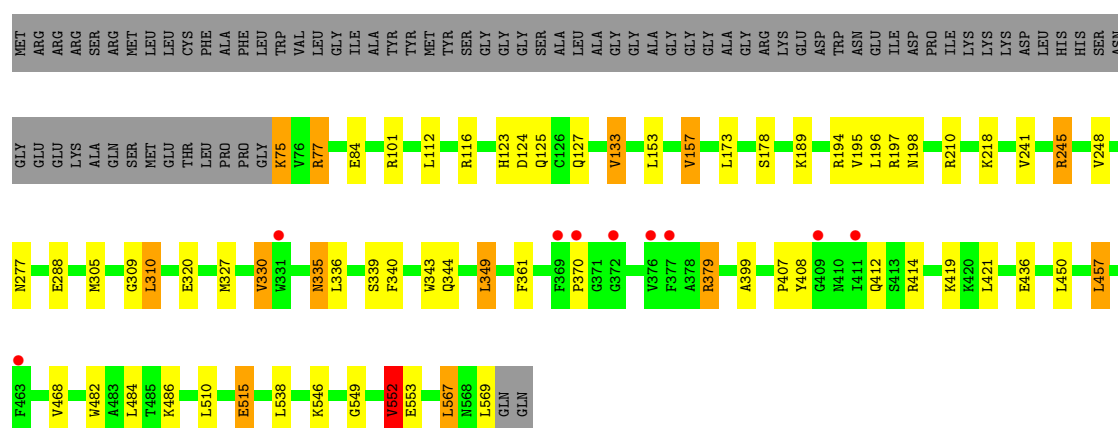
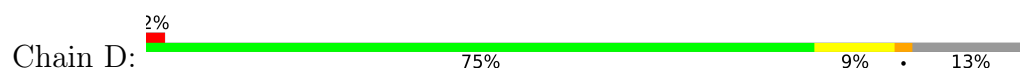


• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

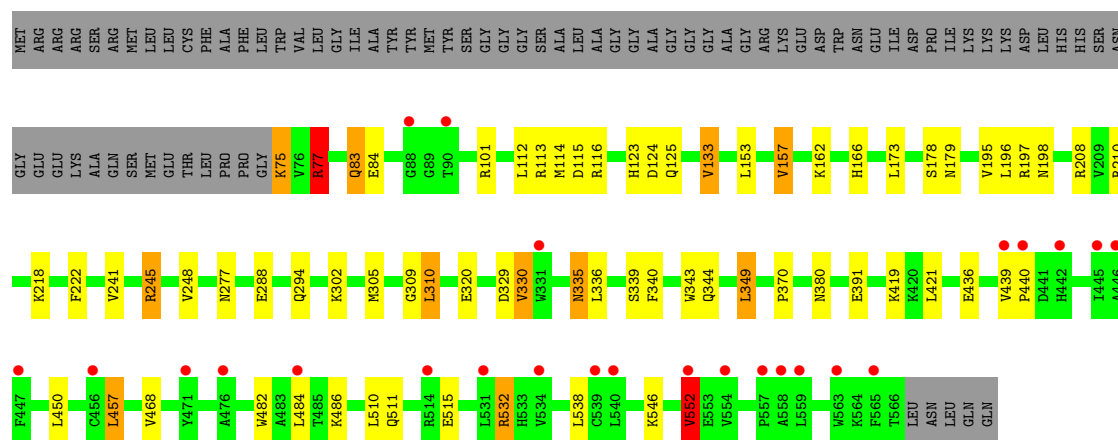
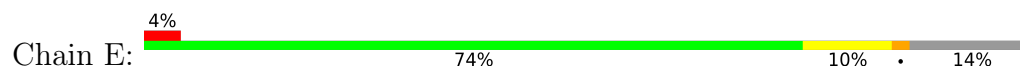




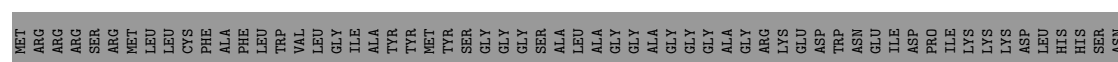
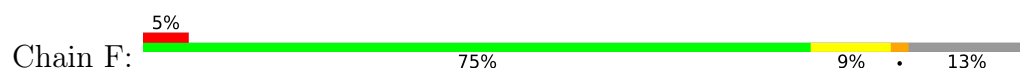
• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

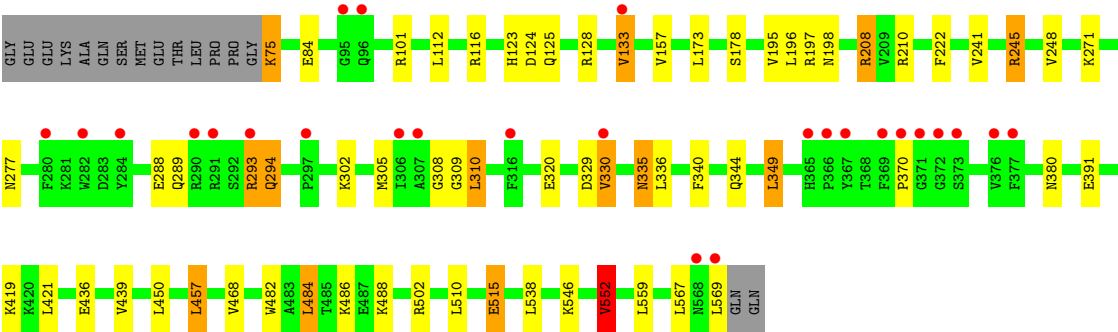


• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2



• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.98Å 123.11Å 248.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.08 – 2.30 124.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (124.08-2.30) 95.3 (124.08-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.213 , 0.251 0.216 , 0.257	Depositor DCC
R_{free} test set	4316 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 21.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24971	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LU2, EDO, UDP, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.90	2/4074 (0.0%)	1.00	7/5510 (0.1%)
1	B	0.93	5/4081 (0.1%)	0.99	5/5517 (0.1%)
1	C	0.96	6/4088 (0.1%)	1.07	13/5527 (0.2%)
1	D	0.98	5/4081 (0.1%)	1.09	9/5517 (0.2%)
1	E	0.91	3/4063 (0.1%)	1.00	5/5493 (0.1%)
1	F	0.96	6/4068 (0.1%)	1.03	12/5501 (0.2%)
All	All	0.94	27/24455 (0.1%)	1.03	51/33065 (0.2%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	75	LYS	CB-CG	-23.48	0.82	1.52
1	F	515	GLU	CB-CG	-22.00	0.86	1.52
1	C	75	LYS	CB-CG	-20.42	0.91	1.52
1	D	515	GLU	CB-CG	-18.22	0.97	1.52
1	C	294	GLN	CB-CG	-16.13	1.04	1.52
1	F	486	LYS	CB-CG	-14.95	1.07	1.52
1	A	294	GLN	CB-CG	-14.89	1.07	1.52
1	D	75	LYS	CB-CG	-14.34	1.09	1.52
1	C	515	GLU	CB-CG	-14.00	1.10	1.52
1	D	486	LYS	CB-CG	-13.19	1.12	1.52
1	B	75	LYS	CB-CG	-12.40	1.15	1.52
1	B	84	GLU	CB-CG	-12.05	1.16	1.52
1	E	294	GLN	CB-CG	-9.61	1.23	1.52
1	B	486	LYS	CB-CG	-8.89	1.25	1.52
1	D	84	GLU	CB-CG	-8.45	1.27	1.52
1	A	486	LYS	CB-CG	8.18	1.76	1.52
1	B	515	GLU	CB-CG	-8.00	1.28	1.52
1	F	294	GLN	CB-CG	-6.31	1.33	1.52
1	F	84	GLU	CB-CG	-6.26	1.33	1.52
1	D	549	GLY	C-O	-6.07	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	75	LYS	CB-CG	-5.71	1.35	1.52
1	C	128	ARG	CA-CB	5.65	1.61	1.53
1	C	130	GLN	CA-CB	5.22	1.62	1.53
1	B	294	GLN	CB-CG	-5.13	1.37	1.52
1	E	440	PRO	C-O	5.11	1.29	1.23
1	C	130	GLN	CA-C	5.09	1.58	1.52
1	F	308	GLY	C-O	5.07	1.29	1.24

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	GLU	CB-CG-CD	27.29	158.99	112.60
1	D	75	LYS	CA-CB-CG	25.84	165.78	114.10
1	D	515	GLU	CA-CB-CG	24.26	162.63	114.10
1	E	75	LYS	CA-CB-CG	20.65	155.40	114.10
1	F	294	GLN	CA-CB-CG	-20.33	73.45	114.10
1	A	75	LYS	CA-CB-CG	16.14	146.39	114.10
1	B	75	LYS	CA-CB-CG	13.68	141.47	114.10
1	F	75	LYS	CA-CB-CG	10.61	135.33	114.10
1	A	84	GLU	CB-CG-CD	9.88	129.40	112.60
1	F	515	GLU	CA-CB-CG	-9.41	95.27	114.10
1	A	486	LYS	CB-CG-CD	-9.26	90.01	111.30
1	C	75	LYS	CB-CG-CD	8.80	131.54	111.30
1	A	294	GLN	CA-CB-CG	-8.58	96.94	114.10
1	F	208	ARG	CB-CG-CD	8.12	129.96	111.30
1	D	515	GLU	CB-CG-CD	-7.72	99.48	112.60
1	C	515	GLU	CA-CB-CG	7.60	129.30	114.10
1	F	294	GLN	CB-CG-CD	-7.57	99.73	112.60
1	F	486	LYS	CB-CG-CD	-7.46	94.13	111.30
1	C	132	ARG	N-CA-C	7.42	126.61	110.80
1	E	77	ARG	NE-CZ-NH2	7.18	125.67	119.20
1	D	84	GLU	CB-CG-CD	6.97	124.45	112.60
1	C	84	GLU	CA-CB-CG	-6.77	100.56	114.10
1	B	486	LYS	CB-CG-CD	-6.62	96.08	111.30
1	E	486	LYS	CA-CB-CG	-6.54	101.03	114.10
1	A	486	LYS	CA-CB-CG	-6.53	101.04	114.10
1	F	133	VAL	CB-CA-C	6.51	117.65	110.62
1	D	486	LYS	CB-CG-CD	-6.50	96.34	111.30
1	D	552	VAL	CB-CA-C	6.46	120.45	110.83
1	C	133	VAL	N-CA-CB	6.36	121.72	111.23
1	A	552	VAL	CB-CA-C	6.30	120.21	110.83
1	A	294	GLN	CB-CG-CD	-6.12	102.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	552	VAL	CB-CA-C	6.06	119.86	110.83
1	F	552	VAL	CB-CA-C	5.97	119.73	110.83
1	E	552	VAL	CB-CA-C	5.95	119.69	110.83
1	E	532	ARG	CA-CB-CG	5.94	125.98	114.10
1	C	552	VAL	CB-CA-C	5.93	119.66	110.83
1	C	294	GLN	CA-CB-CG	5.87	125.84	114.10
1	C	131	TRP	CB-CA-C	-5.76	99.58	111.22
1	F	75	LYS	CB-CG-CD	-5.59	98.43	111.30
1	D	75	LYS	CB-CG-CD	-5.59	98.44	111.30
1	F	293	ARG	NE-CZ-NH1	-5.56	115.94	121.50
1	C	294	GLN	CB-CG-CD	5.56	122.05	112.60
1	D	133	VAL	CB-CA-C	5.43	116.48	110.62
1	F	208	ARG	CG-CD-NE	5.39	123.86	112.00
1	C	135	LEU	CA-CB-CG	5.36	135.07	116.30
1	B	133	VAL	N-CA-CB	-5.30	106.37	112.21
1	C	486	LYS	CB-CG-CD	-5.20	99.35	111.30
1	F	133	VAL	N-CA-CB	-5.16	106.19	112.33
1	D	77	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	B	537	ASN	N-CA-CB	5.04	118.90	111.43
1	C	330	VAL	N-CA-C	5.01	119.75	109.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3976	0	3903	29	0
1	B	3983	0	3916	38	0
1	C	3987	0	3919	27	0
1	D	3983	0	3916	33	0
1	E	3962	0	3887	29	0
1	F	3973	0	3898	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	25	0	11	0	0
3	B	25	0	11	0	0
3	C	25	0	11	0	0
3	D	25	0	11	0	0
3	E	25	0	11	0	0
3	F	25	0	11	0	0
4	A	20	0	30	3	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	1	0
4	E	4	0	6	0	0
4	F	4	0	6	1	0
5	A	21	0	6	5	0
5	B	21	0	7	4	0
5	D	21	0	7	1	0
6	A	194	0	0	5	0
6	B	147	0	0	2	0
6	C	138	0	0	5	0
6	D	163	0	0	6	0
6	E	117	0	0	4	0
6	F	89	0	0	1	0
All	All	24971	0	23585	173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194[B]:ARG:HH21	1:B:194[B]:ARG:CB	1.19	1.54
1:B:194[B]:ARG:NH2	1:B:194[B]:ARG:HB3	1.44	1.29
1:B:194[B]:ARG:HH21	1:B:194[B]:ARG:CG	1.53	1.17
1:B:194[B]:ARG:CB	1:B:194[B]:ARG:NH2	2.01	1.15
1:B:194[B]:ARG:HH21	1:B:194[B]:ARG:HB3	0.90	1.00
1:B:194[B]:ARG:NH2	1:B:194[B]:ARG:CG	2.22	0.86
1:D:327:MET:O	1:D:379[A]:ARG:NH1	2.13	0.81
1:D:414:ARG:HD3	6:D:721:HOH:O	1.81	0.81
1:A:457:LEU:HD13	1:A:482:TRP:CE2	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:LEU:HD13	1:E:482:TRP:CE2	2.18	0.79
1:C:457:LEU:HD13	1:C:482:TRP:CE2	2.18	0.78
1:D:457:LEU:HD13	1:D:482:TRP:CE2	2.18	0.78
1:F:457:LEU:HD13	1:F:482:TRP:CE2	2.19	0.78
1:B:457:LEU:HD13	1:B:482:TRP:CE2	2.18	0.77
1:C:305:MET:HE1	1:C:336:LEU:HD13	1.66	0.77
1:C:438:ARG:NH1	1:C:481:GLU:HG2	2.00	0.76
1:E:305:MET:HE1	1:E:336:LEU:HD13	1.67	0.76
1:B:305:MET:HE1	1:B:336:LEU:HD13	1.67	0.75
1:B:194[B]:ARG:NH2	1:B:194[B]:ARG:HG2	2.02	0.75
1:A:305:MET:HE1	1:A:336:LEU:HD13	1.69	0.75
1:D:305:MET:HE1	1:D:336:LEU:HD13	1.69	0.74
5:A:608:LU2:O3	1:B:463:PHE:HB2	1.88	0.74
1:A:361:PHE:CZ	5:A:608:LU2:H1	2.23	0.73
1:F:305:MET:HE1	1:F:336:LEU:HD13	1.70	0.71
1:D:361:PHE:CZ	5:D:604:LU2:H1	2.26	0.70
5:A:608:LU2:O3	1:B:463:PHE:CD2	2.46	0.69
1:D:194[B]:ARG:HH21	1:D:194[B]:ARG:HG2	1.57	0.68
1:D:194[B]:ARG:HH21	1:D:194[B]:ARG:CG	2.07	0.67
1:D:198:ASN:HD22	1:D:210:ARG:HH11	1.43	0.66
1:C:198:ASN:HD22	1:C:210:ARG:HH11	1.45	0.65
1:B:198:ASN:HD22	1:B:210:ARG:HH11	1.45	0.64
1:A:198:ASN:HD22	1:A:210:ARG:HH11	1.46	0.63
1:B:363:LYS:HG2	5:B:604:LU2:O6	1.99	0.62
1:F:198:ASN:HD22	1:F:210:ARG:HH11	1.45	0.62
1:C:439:VAL:HG12	6:C:761:HOH:O	2.00	0.61
1:C:132:ARG:HD2	1:C:239:GLU:OE1	2.00	0.61
1:C:89:GLY:O	1:D:412:GLN:HG2	2.01	0.60
1:E:198:ASN:HD22	1:E:210:ARG:HH11	1.46	0.60
1:E:115:ASP:OD2	6:E:701:HOH:O	2.16	0.60
1:C:132:ARG:CD	1:C:239:GLU:OE1	2.50	0.60
1:A:463:PHE:CD2	5:B:604:LU2:O3	2.57	0.58
1:C:554:VAL:HG13	6:C:741:HOH:O	2.04	0.57
1:E:77:ARG:HD2	6:E:794:HOH:O	2.03	0.57
1:E:179:ASN:HB3	1:F:128:ARG:HB3	1.88	0.56
1:D:194[B]:ARG:HB3	1:D:194[B]:ARG:NH2	2.21	0.56
5:A:608:LU2:O3	1:B:463:PHE:CB	2.53	0.56
1:A:252:ILE:HG12	4:A:603:EDO:H11	1.88	0.55
1:E:329:ASP:H	1:E:380:ASN:HD21	1.55	0.55
1:C:538:LEU:HB3	1:C:552:VAL:HG22	1.90	0.54
1:B:329:ASP:H	1:B:380:ASN:HD21	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:HIS:HD2	1:A:125:GLN:H	1.56	0.53
1:C:329:ASP:H	1:C:380:ASN:HD21	1.56	0.53
1:A:538:LEU:HB3	1:A:552:VAL:HG22	1.90	0.53
1:E:123:HIS:HD2	1:E:125:GLN:H	1.57	0.53
1:F:538:LEU:HB3	1:F:552:VAL:HG22	1.91	0.53
1:A:329:ASP:H	1:A:380:ASN:HD21	1.57	0.52
1:D:178:SER:O	1:D:197:ARG:NH2	2.43	0.52
1:B:554:VAL:HG13	6:B:725:HOH:O	2.10	0.52
1:E:538:LEU:HB3	1:E:552:VAL:HG22	1.90	0.52
1:F:178:SER:O	1:F:197:ARG:NH2	2.42	0.52
1:E:178:SER:O	1:E:197:ARG:NH2	2.42	0.52
1:A:414:ARG:HD3	6:A:712:HOH:O	2.08	0.51
1:B:178:SER:O	1:B:197:ARG:NH2	2.43	0.51
1:D:123:HIS:HD2	1:D:125:GLN:H	1.58	0.51
1:A:178:SER:O	1:A:197:ARG:NH2	2.43	0.51
1:B:538:LEU:HB3	1:B:552:VAL:HG22	1.93	0.51
1:A:359:HIS:CE1	4:A:605:EDO:H22	2.46	0.51
1:B:123:HIS:HD2	1:B:125:GLN:H	1.59	0.51
1:D:194[B]:ARG:HH21	1:D:194[B]:ARG:HB3	1.76	0.50
1:F:329:ASP:H	1:F:380:ASN:HD21	1.57	0.50
1:B:516:ASP:HB2	1:E:113:ARG:CZ	2.42	0.50
1:D:538:LEU:HB3	1:D:552:VAL:HG22	1.92	0.50
1:C:178:SER:O	1:C:197:ARG:NH2	2.42	0.50
1:B:516:ASP:HB2	1:E:113:ARG:NH2	2.27	0.50
1:D:399:ALA:HB2	1:D:567:LEU:HD22	1.93	0.50
1:C:123:HIS:HD2	1:C:125:GLN:H	1.60	0.50
1:A:399:ALA:HB2	1:A:567:LEU:HD22	1.94	0.49
1:E:511:GLN:NE2	6:E:704:HOH:O	2.36	0.49
1:A:248:VAL:HB	1:A:349:LEU:HD12	1.95	0.49
1:D:248:VAL:HB	1:D:349:LEU:HD12	1.95	0.49
1:B:399:ALA:HB2	1:B:567:LEU:HD22	1.94	0.49
1:D:407:PRO:HA	6:D:845:HOH:O	2.12	0.48
1:E:248:VAL:HB	1:E:349:LEU:HD12	1.95	0.48
1:F:123:HIS:HD2	1:F:125:GLN:H	1.59	0.48
1:D:414:ARG:CD	6:D:721:HOH:O	2.51	0.48
1:B:194[B]:ARG:HB3	1:B:194[B]:ARG:HH22	1.61	0.48
1:C:248:VAL:HB	1:C:349:LEU:HD12	1.95	0.48
1:B:131:TRP:CH2	1:B:236:PRO:HG3	2.49	0.47
1:B:248:VAL:HB	1:B:349:LEU:HD12	1.95	0.47
1:D:553:GLU:CG	6:D:723:HOH:O	2.62	0.47
1:E:133:VAL:HG13	1:E:166:HIS:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ILE:HG12	4:A:603:EDO:C1	2.43	0.47
1:E:162:LYS:HE2	6:E:720:HOH:O	2.15	0.47
1:D:194[B]:ARG:HH21	1:D:194[B]:ARG:CB	2.27	0.47
5:A:608:LU2:O3	1:B:463:PHE:CG	2.68	0.47
1:D:127:GLN:HB2	6:D:808:HOH:O	2.13	0.47
1:F:248:VAL:HB	1:F:349:LEU:HD12	1.97	0.47
1:B:245:ARG:NH1	1:B:320:GLU:OE2	2.47	0.47
1:D:245:ARG:NH1	1:D:320:GLU:OE2	2.48	0.47
1:D:553:GLU:HG2	6:D:723:HOH:O	2.15	0.46
1:E:198:ASN:ND2	1:E:210:ARG:HH11	2.13	0.46
1:C:245:ARG:NH1	1:C:320:GLU:OE2	2.48	0.46
1:C:132:ARG:CG	1:C:135:LEU:HD13	2.46	0.46
1:B:340:PHE:HB3	1:B:344:GLN:NE2	2.31	0.46
1:F:309:GLY:C	1:F:310:LEU:HD23	2.41	0.46
1:C:309:GLY:C	1:C:310:LEU:HD23	2.41	0.45
1:D:309:GLY:C	1:D:310:LEU:HD23	2.40	0.45
1:A:162:LYS:HE2	6:A:778:HOH:O	2.16	0.45
1:F:208:ARG:HD2	1:F:222:PHE:CD1	2.51	0.45
1:F:245:ARG:NH1	1:F:320:GLU:OE2	2.49	0.45
1:E:340:PHE:HB3	1:E:344:GLN:NE2	2.32	0.45
1:A:213:ASP:HB3	4:D:603:EDO:H21	1.97	0.45
1:A:545:ALA:O	6:A:701:HOH:O	2.21	0.45
1:B:309:GLY:C	1:B:310:LEU:HD23	2.42	0.45
1:A:198:ASN:ND2	1:A:210:ARG:HH11	2.14	0.45
1:A:288:GLU:HG2	6:A:884:HOH:O	2.16	0.45
1:F:198:ASN:ND2	1:F:210:ARG:HH11	2.13	0.45
1:A:457:LEU:HD13	1:A:482:TRP:CD2	2.52	0.44
1:F:457:LEU:HD13	1:F:482:TRP:CD2	2.52	0.44
1:F:484:LEU:HD11	4:F:603:EDO:H21	2.00	0.44
1:D:335:ASN:HD22	1:D:335:ASN:H	1.66	0.44
1:C:153:LEU:O	1:C:157:VAL:HG13	2.18	0.44
1:A:309:GLY:C	1:A:310:LEU:HD23	2.43	0.44
1:B:198:ASN:ND2	1:B:210:ARG:HH11	2.14	0.44
1:C:340:PHE:HB3	1:C:344:GLN:NE2	2.33	0.44
1:E:309:GLY:C	1:E:310:LEU:HD23	2.43	0.44
1:C:183:ASP:HB2	6:C:772:HOH:O	2.17	0.43
1:C:457:LEU:HD13	1:C:482:TRP:CD2	2.53	0.43
1:D:198:ASN:ND2	1:D:210:ARG:HH11	2.12	0.43
1:B:323:LYS:O	6:B:701:HOH:O	2.21	0.43
1:E:83[A]:GLN:HE21	1:E:83[A]:GLN:HB2	1.57	0.43
1:A:340:PHE:HB3	1:A:344:GLN:NE2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:ASN:H	1:E:335:ASN:HD22	1.67	0.43
1:B:153:LEU:O	1:B:157:VAL:HG13	2.18	0.43
1:B:335:ASN:H	1:B:335:ASN:HD22	1.66	0.43
1:B:457:LEU:HD13	1:B:482:TRP:CD2	2.52	0.43
1:D:340:PHE:HB3	1:D:344:GLN:NE2	2.34	0.43
1:D:457:LEU:HD13	1:D:482:TRP:CD2	2.52	0.43
1:B:363:LYS:CG	5:B:604:LU2:O6	2.66	0.43
1:A:245:ARG:NH1	1:A:320:GLU:OE2	2.51	0.43
1:C:438:ARG:NH1	6:C:707:HOH:O	2.51	0.43
1:E:335:ASN:HD22	1:E:335:ASN:N	2.17	0.43
1:E:457:LEU:HD13	1:E:482:TRP:CD2	2.53	0.43
1:A:153:LEU:O	1:A:157:VAL:HG13	2.18	0.43
1:B:335:ASN:HD22	1:B:335:ASN:N	2.17	0.43
1:F:340:PHE:HB3	1:F:344:GLN:NE2	2.34	0.43
1:E:153:LEU:O	1:E:157:VAL:HG13	2.19	0.43
1:A:133:VAL:HG13	1:A:166:HIS:CE1	2.54	0.42
1:C:335:ASN:HD22	1:C:335:ASN:N	2.17	0.42
1:F:320:GLU:HB2	6:F:781:HOH:O	2.19	0.42
1:A:335:ASN:HD22	1:A:335:ASN:N	2.17	0.42
1:D:335:ASN:HD22	1:D:335:ASN:N	2.17	0.42
1:F:271:LYS:HD3	1:F:289[A]:GLN:HE22	1.85	0.42
1:B:305:MET:HE2	1:B:339:SER:HB2	2.02	0.42
1:C:335:ASN:HD22	1:C:335:ASN:H	1.66	0.42
1:F:335:ASN:N	1:F:335:ASN:HD22	2.18	0.42
1:E:245:ARG:NH1	1:E:320:GLU:OE2	2.52	0.42
1:E:83[A]:GLN:OE1	1:E:114:MET:HG2	2.19	0.42
1:A:335:ASN:HD22	1:A:335:ASN:H	1.67	0.41
1:C:198:ASN:ND2	1:C:210:ARG:HH11	2.13	0.41
1:D:379[A]:ARG:HG3	1:D:408:TYR:HA	2.02	0.41
1:C:192:LYS:NZ	6:C:708:HOH:O	2.52	0.41
1:A:442:HIS:HB2	6:A:871:HOH:O	2.21	0.41
5:B:604:LU2:H15	5:B:604:LU2:H8	1.72	0.41
1:D:153:LEU:O	1:D:157:VAL:HG13	2.20	0.41
1:E:343:TRP:CD1	1:E:349:LEU:HD22	2.56	0.41
1:B:208:ARG:HD3	1:B:222:PHE:CD1	2.56	0.40
1:C:343:TRP:CD1	1:C:349:LEU:HD22	2.56	0.40
1:D:305:MET:HE2	1:D:339:SER:HB2	2.03	0.40
1:D:343:TRP:CD1	1:D:349:LEU:HD22	2.56	0.40
1:E:208:ARG:HD3	1:E:222:PHE:CD1	2.56	0.40
1:E:305:MET:HE2	1:E:339:SER:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/571 (87%)	481 (97%)	12 (2%)	2 (0%)	30	38
1	B	495/571 (87%)	478 (97%)	15 (3%)	2 (0%)	30	38
1	C	496/571 (87%)	479 (97%)	13 (3%)	4 (1%)	16	20
1	D	495/571 (87%)	481 (97%)	12 (2%)	2 (0%)	30	38
1	E	493/571 (86%)	478 (97%)	13 (3%)	2 (0%)	30	38
1	F	494/571 (86%)	479 (97%)	13 (3%)	2 (0%)	30	38
All	All	2968/3426 (87%)	2876 (97%)	78 (3%)	14 (0%)	24	31

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	VAL
1	B	330	VAL
1	C	133	VAL
1	C	330	VAL
1	D	330	VAL
1	E	330	VAL
1	F	330	VAL
1	A	370	PRO
1	B	370	PRO
1	C	370	PRO
1	D	370	PRO
1	E	370	PRO
1	F	370	PRO
1	C	557	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/485 (89%)	392 (91%)	38 (9%)	9	12
1	B	430/485 (89%)	393 (91%)	37 (9%)	10	13
1	C	431/485 (89%)	392 (91%)	39 (9%)	9	12
1	D	430/485 (89%)	394 (92%)	36 (8%)	10	14
1	E	428/485 (88%)	390 (91%)	38 (9%)	9	12
1	F	429/485 (88%)	391 (91%)	38 (9%)	9	12
All	All	2578/2910 (89%)	2352 (91%)	226 (9%)	9	12

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	77	ARG
1	A	84	GLU
1	A	101	ARG
1	A	112	LEU
1	A	116	ARG
1	A	124	ASP
1	A	133	VAL
1	A	157	VAL
1	A	173	LEU
1	A	195	VAL
1	A	196	LEU
1	A	218	LYS
1	A	241	VAL
1	A	245	ARG
1	A	277	ASN
1	A	288	GLU
1	A	302	LYS
1	A	310	LEU
1	A	327	MET
1	A	330	VAL
1	A	335	ASN
1	A	349	LEU
1	A	419	LYS
1	A	421	LEU
1	A	436	GLU
1	A	439	VAL

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Mol	Chain	Res	Type
1	A	450	LEU
1	A	457	LEU
1	A	468	VAL
1	A	484	LEU
1	A	510	LEU
1	A	514	ARG
1	A	515	GLU
1	A	546	LYS
1	A	552	VAL
1	A	567	LEU
1	A	569	LEU
1	B	84	GLU
1	B	101	ARG
1	B	112	LEU
1	B	116	ARG
1	B	124	ASP
1	B	127	GLN
1	B	128	ARG
1	B	133	VAL
1	B	157	VAL
1	B	173	LEU
1	B	195	VAL
1	B	241	VAL
1	B	245	ARG
1	B	271	LYS
1	B	277	ASN
1	B	288	GLU
1	B	302	LYS
1	B	310	LEU
1	B	330	VAL
1	B	335	ASN
1	B	349	LEU
1	B	419	LYS
1	B	421	LEU
1	B	436	GLU
1	B	439	VAL
1	B	450	LEU
1	B	457	LEU
1	B	468	VAL
1	B	484	LEU
1	B	486	LYS
1	B	488	LYS

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Mol	Chain	Res	Type
1	B	510	LEU
1	B	537	ASN
1	B	546	LYS
1	B	552	VAL
1	B	567	LEU
1	B	569	LEU
1	C	75	LYS
1	C	84	GLU
1	C	112	LEU
1	C	116	ARG
1	C	124	ASP
1	C	128	ARG
1	C	131	TRP
1	C	133	VAL
1	C	135	LEU
1	C	157	VAL
1	C	173	LEU
1	C	195	VAL
1	C	196	LEU
1	C	239	GLU
1	C	241	VAL
1	C	245	ARG
1	C	277	ASN
1	C	288	GLU
1	C	302	LYS
1	C	310	LEU
1	C	330	VAL
1	C	335	ASN
1	C	349	LEU
1	C	419	LYS
1	C	421	LEU
1	C	436	GLU
1	C	438	ARG
1	C	439	VAL
1	C	450	LEU
1	C	451	GLN
1	C	457	LEU
1	C	468	VAL
1	C	484	LEU
1	C	502	ARG
1	C	510	LEU
1	C	546	LYS

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Mol	Chain	Res	Type
1	C	552	VAL
1	C	567	LEU
1	C	569	LEU
1	D	75	LYS
1	D	77	ARG
1	D	101	ARG
1	D	112	LEU
1	D	116	ARG
1	D	124	ASP
1	D	133	VAL
1	D	157	VAL
1	D	173	LEU
1	D	189	LYS
1	D	195	VAL
1	D	196	LEU
1	D	218	LYS
1	D	241	VAL
1	D	245	ARG
1	D	277	ASN
1	D	288	GLU
1	D	310	LEU
1	D	330	VAL
1	D	335	ASN
1	D	349	LEU
1	D	379[A]	ARG
1	D	379[B]	ARG
1	D	419	LYS
1	D	421	LEU
1	D	436	GLU
1	D	450	LEU
1	D	457	LEU
1	D	468	VAL
1	D	484	LEU
1	D	510	LEU
1	D	515	GLU
1	D	546	LYS
1	D	552	VAL
1	D	567	LEU
1	D	569	LEU
1	E	75	LYS
1	E	77	ARG
1	E	83[A]	GLN

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Mol	Chain	Res	Type
1	E	83[B]	GLN
1	E	84	GLU
1	E	101	ARG
1	E	112	LEU
1	E	116	ARG
1	E	124	ASP
1	E	133	VAL
1	E	157	VAL
1	E	173	LEU
1	E	195	VAL
1	E	196	LEU
1	E	218	LYS
1	E	241	VAL
1	E	245	ARG
1	E	277	ASN
1	E	288	GLU
1	E	302	LYS
1	E	310	LEU
1	E	330	VAL
1	E	335	ASN
1	E	349	LEU
1	E	391	GLU
1	E	419	LYS
1	E	421	LEU
1	E	436	GLU
1	E	439	VAL
1	E	450	LEU
1	E	457	LEU
1	E	468	VAL
1	E	484	LEU
1	E	510	LEU
1	E	515	GLU
1	E	532	ARG
1	E	546	LYS
1	E	552	VAL
1	F	75	LYS
1	F	101	ARG
1	F	112	LEU
1	F	116	ARG
1	F	124	ASP
1	F	133	VAL
1	F	157	VAL

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Mol	Chain	Res	Type
1	F	173	LEU
1	F	195	VAL
1	F	196	LEU
1	F	241	VAL
1	F	245	ARG
1	F	277	ASN
1	F	288	GLU
1	F	294	GLN
1	F	302	LYS
1	F	310	LEU
1	F	330	VAL
1	F	335	ASN
1	F	349	LEU
1	F	391	GLU
1	F	419	LYS
1	F	421	LEU
1	F	436	GLU
1	F	439	VAL
1	F	450	LEU
1	F	457	LEU
1	F	468	VAL
1	F	484	LEU
1	F	488	LYS
1	F	502	ARG
1	F	510	LEU
1	F	515	GLU
1	F	546	LYS
1	F	552	VAL
1	F	559	LEU
1	F	567	LEU
1	F	569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	102	ASN
1	A	106	GLN
1	A	123	HIS
1	A	125	GLN
1	A	127	GLN
1	A	198	ASN

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Mol	Chain	Res	Type
1	A	277	ASN
1	A	296	ASN
1	A	335	ASN
1	A	344	GLN
1	A	365	HIS
1	A	380	ASN
1	A	462	HIS
1	A	524	GLN
1	A	537	ASN
1	A	568	ASN
1	B	96	GLN
1	B	106	GLN
1	B	123	HIS
1	B	125	GLN
1	B	198	ASN
1	B	262	GLN
1	B	277	ASN
1	B	296	ASN
1	B	335	ASN
1	B	344	GLN
1	B	365	HIS
1	B	380	ASN
1	B	451	GLN
1	B	462	HIS
1	B	524	GLN
1	B	568	ASN
1	C	96	GLN
1	C	102	ASN
1	C	106	GLN
1	C	123	HIS
1	C	125	GLN
1	C	127	GLN
1	C	166	HIS
1	C	198	ASN
1	C	277	ASN
1	C	296	ASN
1	C	335	ASN
1	C	344	GLN
1	C	365	HIS
1	C	380	ASN
1	C	432	ASN
1	C	462	HIS

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Mol	Chain	Res	Type
1	C	537	ASN
1	C	568	ASN
1	D	123	HIS
1	D	125	GLN
1	D	127	GLN
1	D	198	ASN
1	D	277	ASN
1	D	296	ASN
1	D	335	ASN
1	D	344	GLN
1	D	365	HIS
1	D	432	ASN
1	D	462	HIS
1	D	524	GLN
1	D	537	ASN
1	D	568	ASN
1	E	96	GLN
1	E	123	HIS
1	E	125	GLN
1	E	127	GLN
1	E	198	ASN
1	E	277	ASN
1	E	296	ASN
1	E	335	ASN
1	E	344	GLN
1	E	365	HIS
1	E	380	ASN
1	E	462	HIS
1	E	537	ASN
1	F	96	GLN
1	F	102	ASN
1	F	106	GLN
1	F	123	HIS
1	F	125	GLN
1	F	127	GLN
1	F	198	ASN
1	F	216	GLN
1	F	277	ASN
1	F	296	ASN
1	F	335	ASN
1	F	344	GLN
1	F	365	HIS

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Mol	Chain	Res	Type
1	F	380	ASN
1	F	451	GLN
1	F	462	HIS
1	F	524	GLN
1	F	537	ASN
1	F	568	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 6 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	UDP	B	602	2	25,26,26	1.26	2 (8%)	38,40,40	1.45	6 (15%)
3	UDP	F	602	2	25,26,26	1.28	4 (16%)	38,40,40	1.82	9 (23%)
4	EDO	A	607	-	3,3,3	0.43	0	2,2,2	0.35	0
4	EDO	B	603	-	3,3,3	0.23	0	2,2,2	0.52	0
3	UDP	C	602	2	25,26,26	1.14	3 (12%)	38,40,40	1.97	7 (18%)
4	EDO	A	604	-	3,3,3	1.03	0	2,2,2	0.29	0
4	EDO	F	603	-	3,3,3	0.49	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	606	-	3,3,3	0.66	0	2,2,2	0.17	0
3	UDP	D	602	2	25,26,26	1.29	3 (12%)	38,40,40	1.76	8 (21%)
4	EDO	D	603	-	3,3,3	1.08	0	2,2,2	0.04	0
5	LU2	D	604	-	23,23,23	1.71	4 (17%)	34,34,34	3.16	13 (38%)
5	LU2	A	608	-	23,23,23	2.32	10 (43%)	34,34,34	3.85	18 (52%)
5	LU2	B	604	-	23,23,23	1.96	9 (39%)	34,34,34	3.06	16 (47%)
3	UDP	A	602	2	25,26,26	1.08	1 (4%)	38,40,40	1.53	7 (18%)
4	EDO	A	605	-	3,3,3	0.79	0	2,2,2	0.27	0
4	EDO	C	603	-	3,3,3	0.53	0	2,2,2	0.23	0
4	EDO	A	603	-	3,3,3	1.38	0	2,2,2	1.29	0
3	UDP	E	602	2	25,26,26	1.35	6 (24%)	38,40,40	1.52	5 (13%)
4	EDO	E	603	-	3,3,3	0.73	0	2,2,2	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	B	602	2	-	1/16/32/32	0/2/2/2
3	UDP	F	602	2	-	1/16/32/32	0/2/2/2
4	EDO	A	607	-	-	1/1/1/1	-
4	EDO	B	603	-	-	1/1/1/1	-
3	UDP	C	602	2	-	0/16/32/32	0/2/2/2
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	F	603	-	-	1/1/1/1	-
4	EDO	A	606	-	-	1/1/1/1	-
3	UDP	D	602	2	-	1/16/32/32	0/2/2/2
4	EDO	D	603	-	-	1/1/1/1	-
5	LU2	D	604	-	-	4/4/4/4	0/3/3/3
5	LU2	A	608	-	-	3/4/4/4	0/3/3/3
5	LU2	B	604	-	-	0/4/4/4	0/3/3/3
3	UDP	A	602	2	-	2/16/32/32	0/2/2/2
4	EDO	A	605	-	-	1/1/1/1	-
4	EDO	C	603	-	-	1/1/1/1	-
4	EDO	A	603	-	-	1/1/1/1	-
3	UDP	E	602	2	-	1/16/32/32	0/2/2/2
4	EDO	E	603	-	-	1/1/1/1	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	604	LU2	C8-C7	-4.74	1.34	1.44
5	A	608	LU2	C8-C7	-4.55	1.35	1.44
5	D	604	LU2	C10-C9	-4.36	1.38	1.48
5	D	604	LU2	C8-C7	-4.29	1.35	1.44
5	A	608	LU2	C5-C7	-4.13	1.36	1.46
5	A	608	LU2	O4-C6	3.73	1.44	1.38
3	B	602	UDP	PA-O3A	3.34	1.63	1.59
5	A	608	LU2	O4-C9	3.31	1.41	1.36
5	A	608	LU2	C3-C2	-3.30	1.34	1.39
5	A	608	LU2	C10-C9	-3.25	1.40	1.48
5	B	604	LU2	C1-C2	3.08	1.43	1.39
3	F	602	UDP	C5-C4	-3.05	1.37	1.43
3	E	602	UDP	O2-C2	3.03	1.28	1.23
5	B	604	LU2	C5-C7	-2.99	1.39	1.46
3	D	602	UDP	C2-N3	-2.89	1.32	1.38
5	A	608	LU2	C15-C10	2.86	1.43	1.39
5	B	604	LU2	O4-C6	2.75	1.42	1.38
5	B	604	LU2	C10-C9	-2.75	1.41	1.48
3	E	602	UDP	C4-N3	-2.72	1.34	1.38
5	B	604	LU2	C15-C10	2.66	1.43	1.39
5	D	604	LU2	C5-C7	-2.64	1.40	1.46
5	A	608	LU2	C3-C4	-2.62	1.35	1.38
5	B	604	LU2	O4-C9	2.61	1.40	1.36
3	E	602	UDP	C2-N1	2.61	1.42	1.38
5	B	604	LU2	C3-C2	-2.44	1.35	1.39
3	C	602	UDP	C5-C4	-2.43	1.38	1.43
3	C	602	UDP	C2-N3	-2.41	1.33	1.38
5	B	604	LU2	C1-C6	2.40	1.42	1.38
3	D	602	UDP	C4-N3	-2.39	1.34	1.38
5	D	604	LU2	C3-C2	-2.28	1.35	1.39
5	A	608	LU2	O3-C7	-2.27	1.19	1.24
3	F	602	UDP	C2-N3	-2.25	1.34	1.38
3	E	602	UDP	C2-N3	-2.22	1.34	1.38
5	A	608	LU2	O5-C12	-2.21	1.31	1.36
3	E	602	UDP	C6-C5	2.15	1.40	1.35
3	D	602	UDP	O4'-C1'	2.14	1.47	1.42
3	F	602	UDP	C4-N3	-2.14	1.34	1.38
3	A	602	UDP	C2-N1	2.12	1.41	1.38
3	B	602	UDP	C5-C4	-2.12	1.39	1.43
3	E	602	UDP	C5-C4	-2.08	1.39	1.43
3	F	602	UDP	C2-N1	2.07	1.41	1.38
3	C	602	UDP	O2-C2	2.05	1.26	1.23

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	608	LU2	O4-C9-C10	10.85	127.01	111.89
5	D	604	LU2	O4-C9-C10	9.86	125.63	111.89
5	A	608	LU2	O4-C6-C1	9.76	129.66	115.83
5	B	604	LU2	O4-C9-C10	8.70	124.01	111.89
5	B	604	LU2	O4-C6-C1	7.99	127.15	115.83
5	B	604	LU2	O3-C7-C8	-6.46	111.54	121.88
5	D	604	LU2	O4-C6-C1	6.30	124.76	115.83
5	D	604	LU2	C11-C10-C9	-6.21	110.20	120.25
3	C	602	UDP	O4-C4-C5	-6.05	114.73	125.16
5	A	608	LU2	C1-C6-C5	-5.90	111.51	121.79
5	A	608	LU2	O3-C7-C8	-5.74	112.69	121.88
3	C	602	UDP	C5-C4-N3	5.65	122.72	114.80
5	A	608	LU2	C4-C5-C6	5.46	122.62	117.41
5	A	608	LU2	C4-C3-C2	-5.39	114.70	119.67
5	D	604	LU2	O3-C7-C8	-5.29	113.41	121.88
3	C	602	UDP	C4-N3-C2	-5.08	120.30	126.61
3	F	602	UDP	O4-C4-C5	-5.07	116.42	125.16
5	A	608	LU2	C5-C7-C8	5.02	125.74	116.31
3	F	602	UDP	C5-C4-N3	4.71	121.39	114.80
5	D	604	LU2	C15-C10-C9	4.56	128.01	120.77
5	A	608	LU2	C9-C8-C7	-4.51	117.50	122.14
3	F	602	UDP	C4-N3-C2	-4.39	121.16	126.61
3	D	602	UDP	C4-N3-C2	-4.33	121.24	126.61
3	E	602	UDP	C5-C4-N3	4.31	120.83	114.80
5	A	608	LU2	C11-C12-C13	4.15	123.73	119.89
3	D	602	UDP	C5-C4-N3	4.06	120.49	114.80
5	D	604	LU2	C10-C9-C8	-3.97	109.89	123.08
3	E	602	UDP	C4-N3-C2	-3.85	121.83	126.61
5	B	604	LU2	C1-C6-C5	-3.84	115.10	121.79
3	B	602	UDP	O4-C4-C5	-3.81	118.59	125.16
5	D	604	LU2	C6-C1-C2	3.77	124.93	118.98
5	D	604	LU2	C3-C4-C5	3.73	125.09	120.92
3	D	602	UDP	O4-C4-C5	-3.56	119.02	125.16
5	A	608	LU2	C6-C1-C2	3.53	124.55	118.98
5	B	604	LU2	O1-C2-C1	3.52	129.07	119.85
5	B	604	LU2	O4-C6-C5	-3.50	117.75	121.19
3	A	602	UDP	O4-C4-C5	-3.45	119.21	125.16
5	A	608	LU2	C15-C14-C13	-3.38	117.12	120.50
5	B	604	LU2	C15-C14-C13	-3.37	117.13	120.50
5	A	608	LU2	C3-C4-C5	3.37	124.69	120.92
5	B	604	LU2	O4-C9-C8	-3.32	118.63	121.70
5	D	604	LU2	C1-C6-C5	-3.32	116.01	121.79
5	D	604	LU2	C9-C8-C7	-3.30	118.75	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	UDP	C5-C4-N3	3.27	119.38	114.80
5	B	604	LU2	C5-C7-C8	3.23	122.36	116.31
5	A	608	LU2	C10-C9-C8	-3.17	112.53	123.08
3	B	602	UDP	C4-N3-C2	-3.17	122.68	126.61
5	A	608	LU2	O1-C2-C3	-3.16	111.59	119.85
5	B	604	LU2	O1-C2-C3	-3.14	111.62	119.85
3	A	602	UDP	O2A-PA-O3A	3.11	115.68	107.27
5	B	604	LU2	C3-C4-C5	3.10	124.39	120.92
3	D	602	UDP	N3-C2-N1	3.08	118.89	114.89
5	D	604	LU2	C5-C7-C8	2.92	121.79	116.31
5	B	604	LU2	C6-C1-C2	2.91	123.56	118.98
3	B	602	UDP	C5-C4-N3	2.88	118.83	114.80
3	A	602	UDP	C4-N3-C2	-2.87	123.05	126.61
3	E	602	UDP	N3-C2-N1	2.86	118.62	114.89
5	A	608	LU2	C10-C11-C12	-2.80	117.65	120.09
3	E	602	UDP	O4-C4-C5	-2.79	120.35	125.16
3	F	602	UDP	O2'-C2'-C1'	2.71	119.45	110.10
3	B	602	UDP	N3-C2-N1	2.70	118.41	114.89
5	B	604	LU2	C14-C13-C12	2.63	122.47	119.66
3	D	602	UDP	O2-C2-N3	-2.62	116.65	121.49
3	F	602	UDP	N3-C2-N1	2.55	118.21	114.89
5	A	608	LU2	O1-C2-C1	2.53	126.48	119.85
5	A	608	LU2	O4-C6-C5	-2.42	118.81	121.19
3	F	602	UDP	O3A-PB-O1B	-2.41	98.35	111.04
5	A	608	LU2	C6-C5-C7	-2.37	117.40	119.60
3	F	602	UDP	O2A-PA-O1A	2.36	123.45	112.44
3	F	602	UDP	O3B-PB-O1B	2.36	120.04	110.83
5	B	604	LU2	C14-C15-C10	2.36	123.32	120.80
5	B	604	LU2	C10-C9-C8	-2.35	115.28	123.08
3	A	602	UDP	O3B-PB-O2B	2.34	116.58	107.80
5	D	604	LU2	C14-C15-C10	-2.34	118.30	120.80
3	C	602	UDP	O2A-PA-O1A	2.31	123.19	112.44
5	B	604	LU2	C4-C5-C6	2.30	119.60	117.41
3	B	602	UDP	O3B-PB-O2B	2.30	116.42	107.80
3	B	602	UDP	O4-C4-N3	2.28	122.58	119.27
3	C	602	UDP	O4-C4-N3	2.26	122.56	119.27
3	A	602	UDP	O3A-PB-O1B	-2.23	99.33	111.04
3	E	602	UDP	O3A-PB-O1B	-2.21	99.42	111.04
3	D	602	UDP	O2B-PB-O1B	2.19	119.38	110.83
3	C	602	UDP	O2'-C2'-C3'	2.18	118.79	111.82
3	A	602	UDP	O2B-PB-O3A	-2.16	97.39	104.64
3	D	602	UDP	O2'-C2'-C1'	2.08	117.26	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	604	LU2	O1-C2-C1	2.08	125.29	119.85
3	D	602	UDP	O3A-PB-O1B	-2.06	100.18	111.04
3	C	602	UDP	N3-C2-N1	2.05	117.56	114.89
3	F	602	UDP	O4-C4-N3	2.00	122.17	119.27

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	604	LU2	C11-C10-C9-O4
5	D	604	LU2	C15-C10-C9-O4
5	D	604	LU2	C11-C10-C9-C8
5	D	604	LU2	C15-C10-C9-C8
5	A	608	LU2	C11-C10-C9-O4
5	A	608	LU2	C15-C10-C9-O4
4	C	603	EDO	O1-C1-C2-O2
4	D	603	EDO	O1-C1-C2-O2
4	A	603	EDO	O1-C1-C2-O2
4	F	603	EDO	O1-C1-C2-O2
3	A	602	UDP	PB-O3A-PA-O2A
4	A	606	EDO	O1-C1-C2-O2
4	A	607	EDO	O1-C1-C2-O2
3	F	602	UDP	O4'-C1'-N1-C6
4	A	605	EDO	O1-C1-C2-O2
4	E	603	EDO	O1-C1-C2-O2
4	B	603	EDO	O1-C1-C2-O2
3	A	602	UDP	PB-O3A-PA-O1A
3	E	602	UDP	PB-O3A-PA-O1A
5	A	608	LU2	C11-C10-C9-C8
3	B	602	UDP	C4'-C5'-O5'-PA
3	D	602	UDP	O4'-C1'-N1-C6

There are no ring outliers.

7 monomers are involved in 15 short contacts:

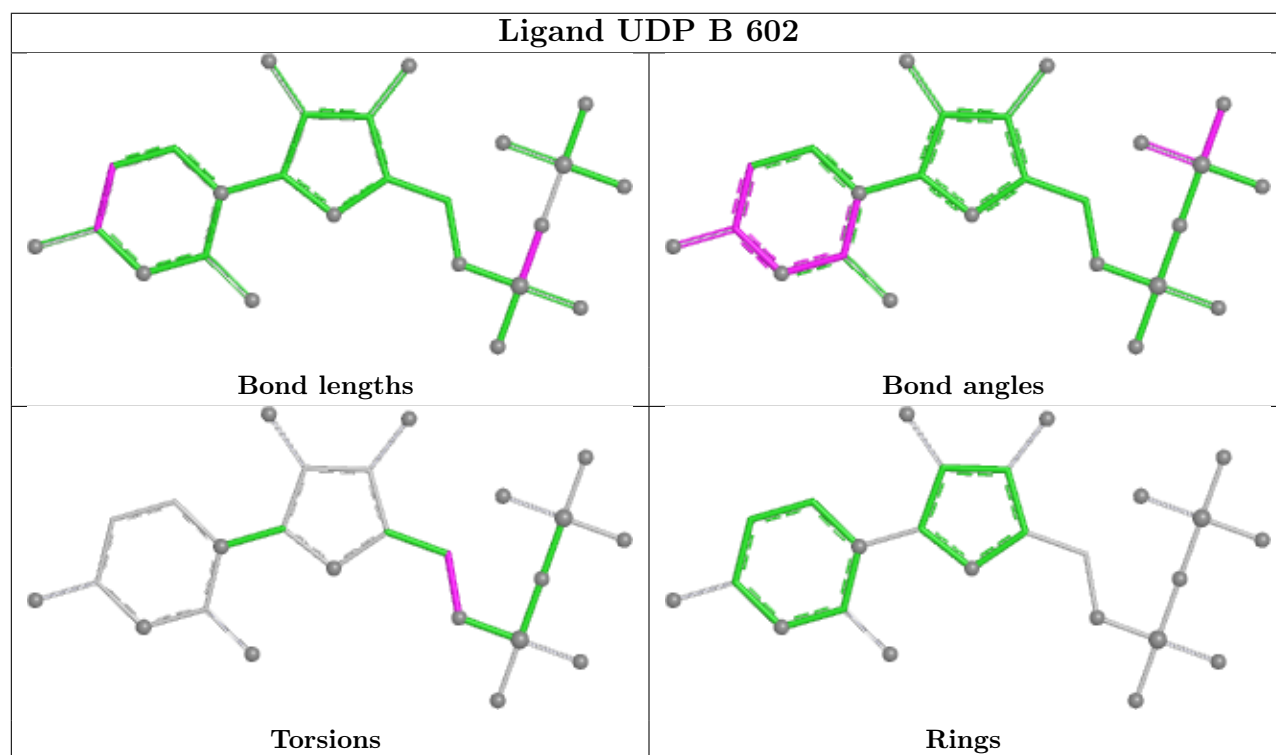
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	603	EDO	1	0
4	D	603	EDO	1	0
5	D	604	LU2	1	0
5	A	608	LU2	5	0
5	B	604	LU2	4	0

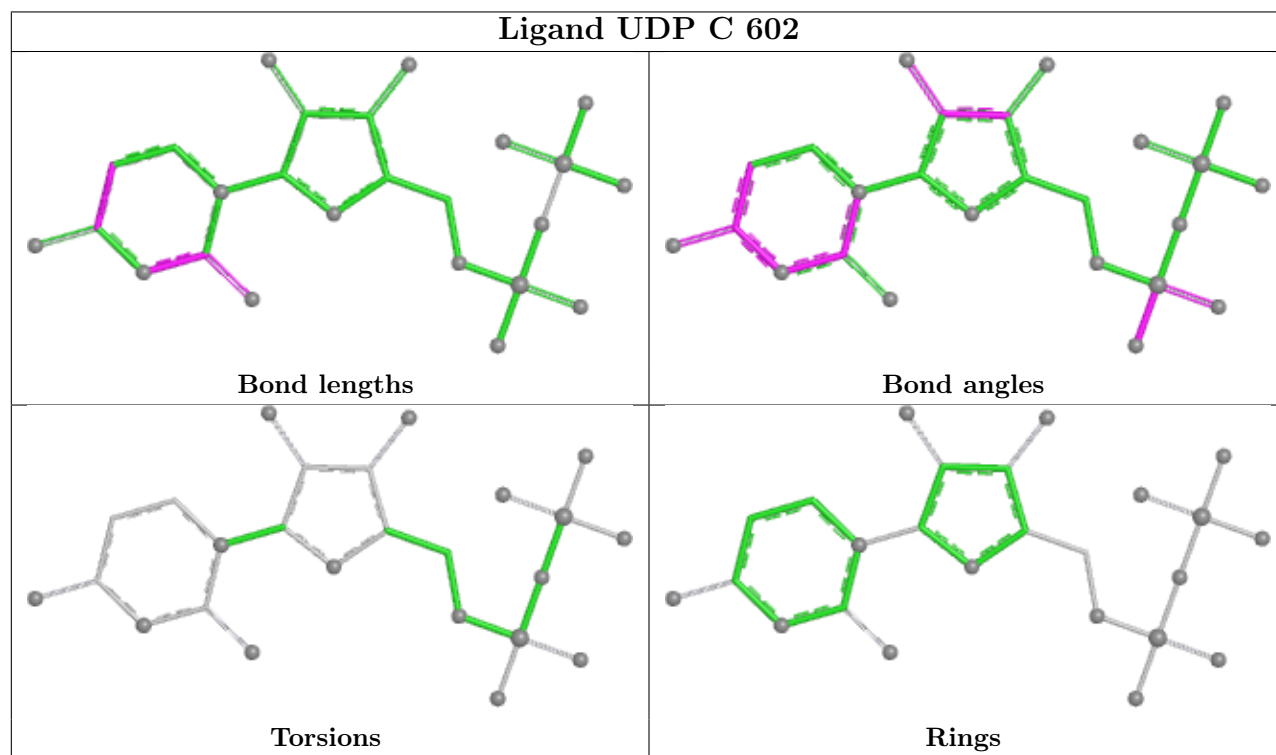
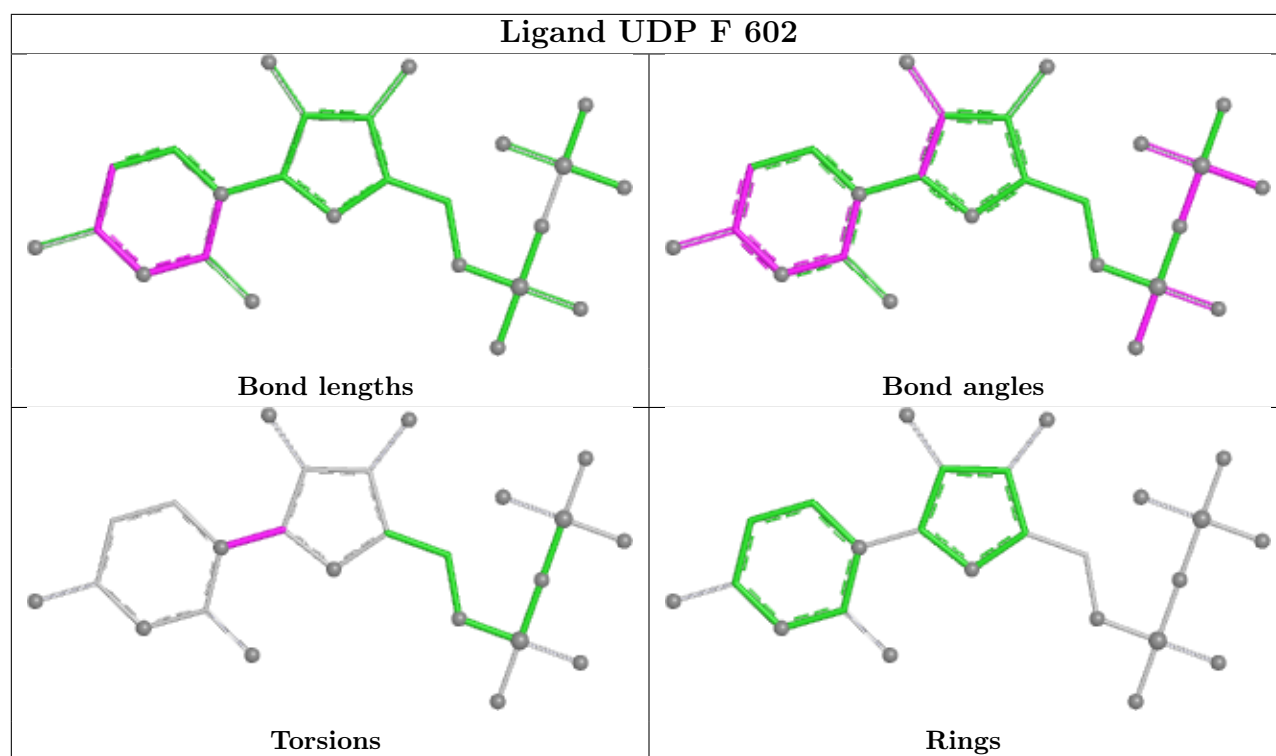
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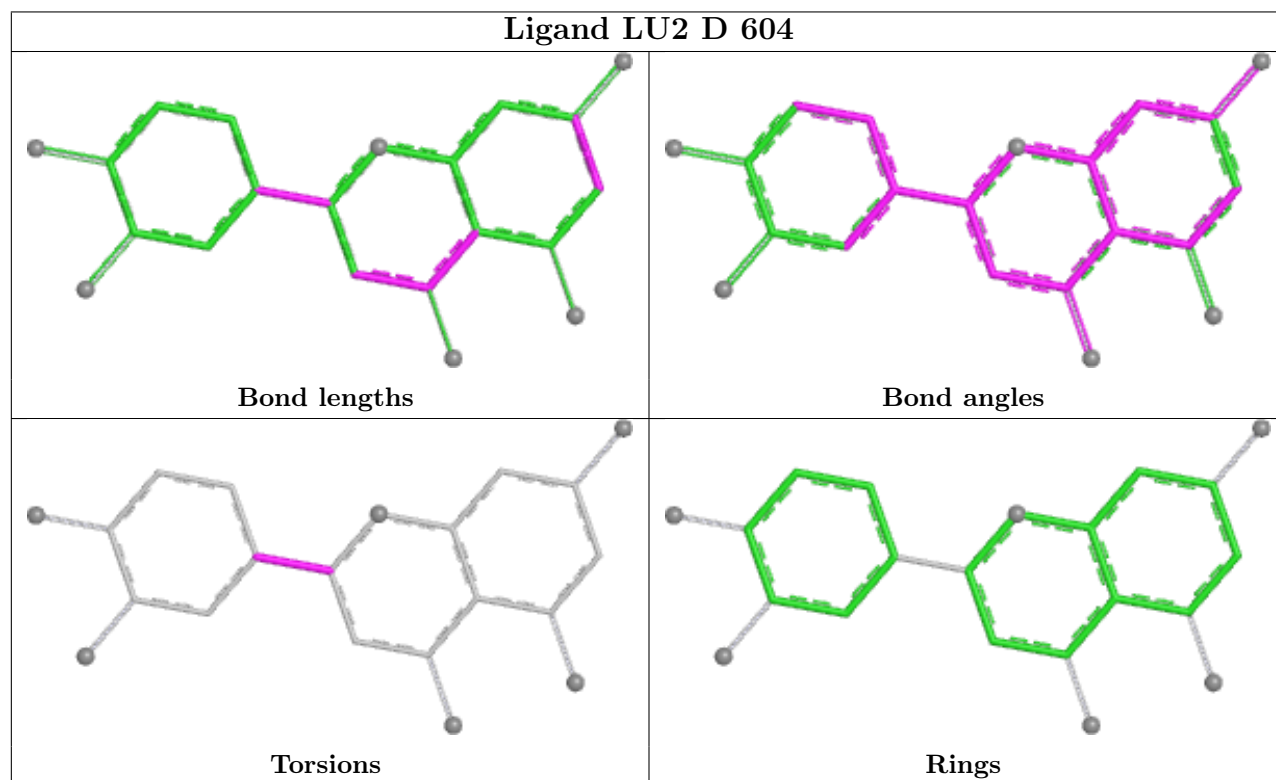
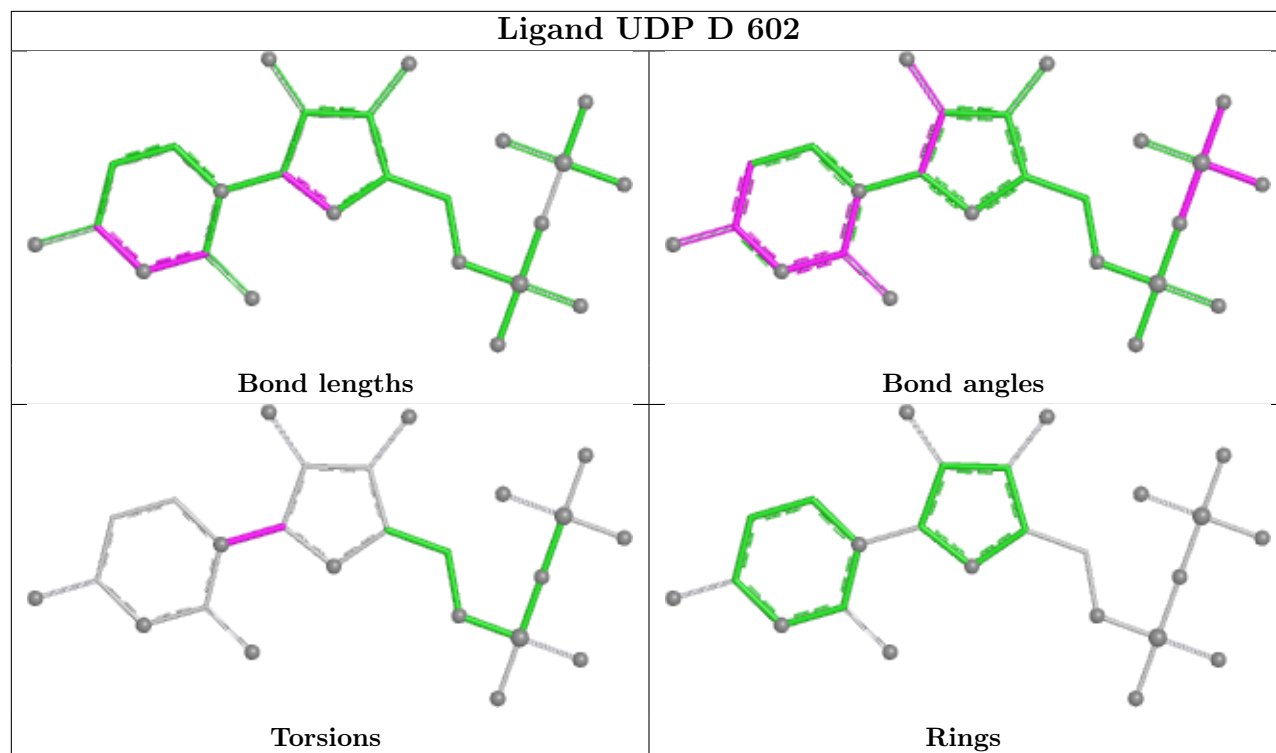
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	EDO	1	0
4	A	603	EDO	2	0

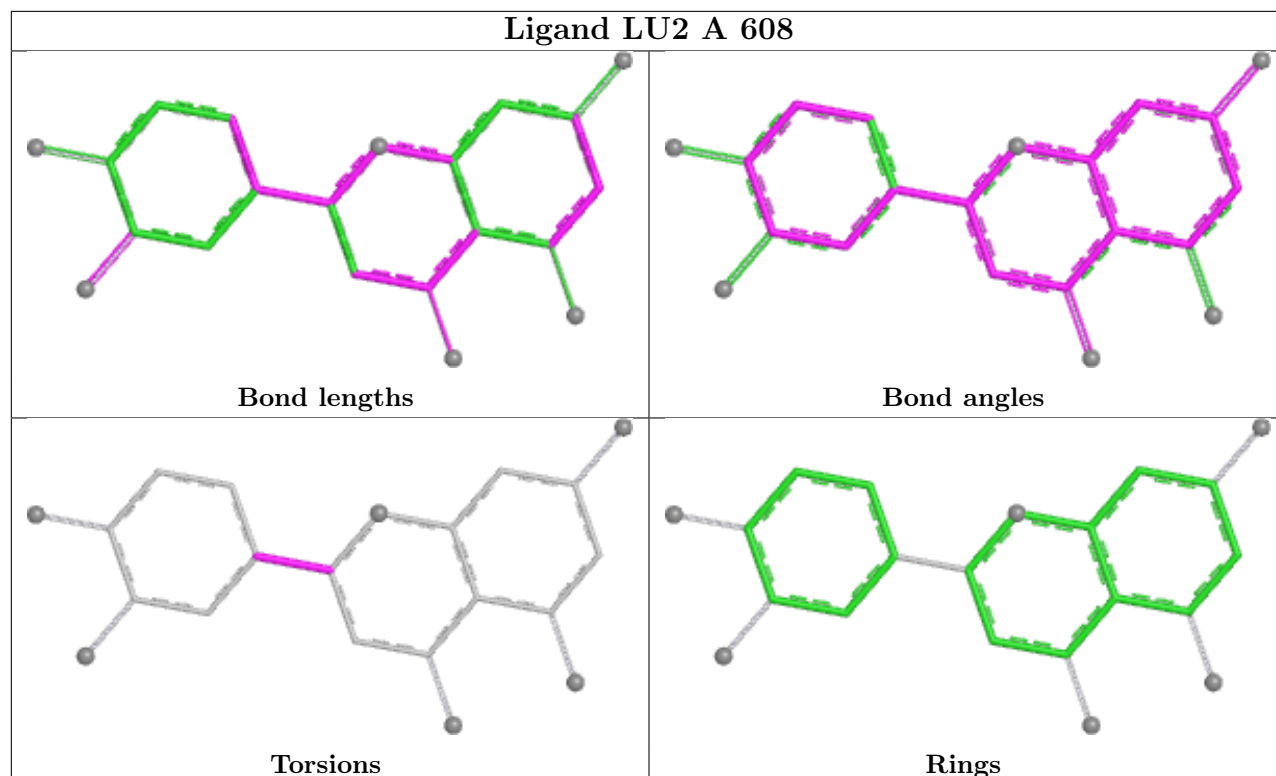
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



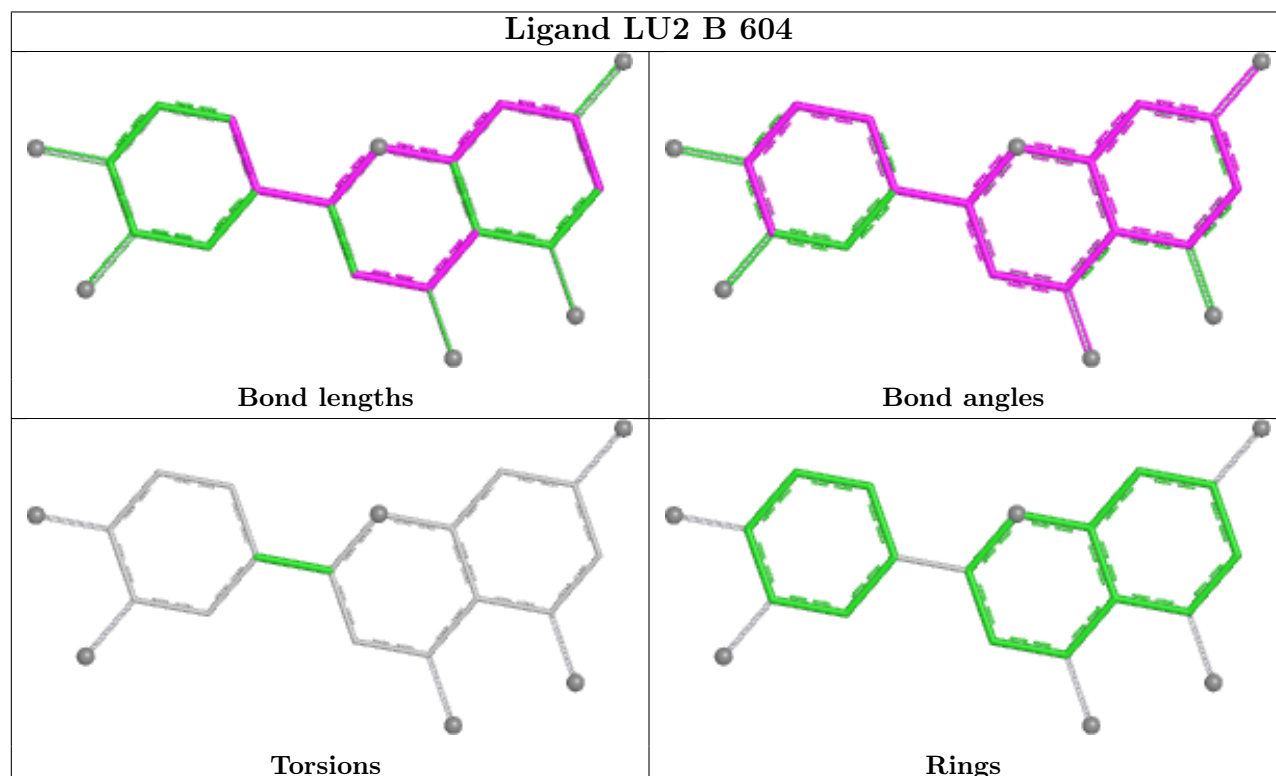


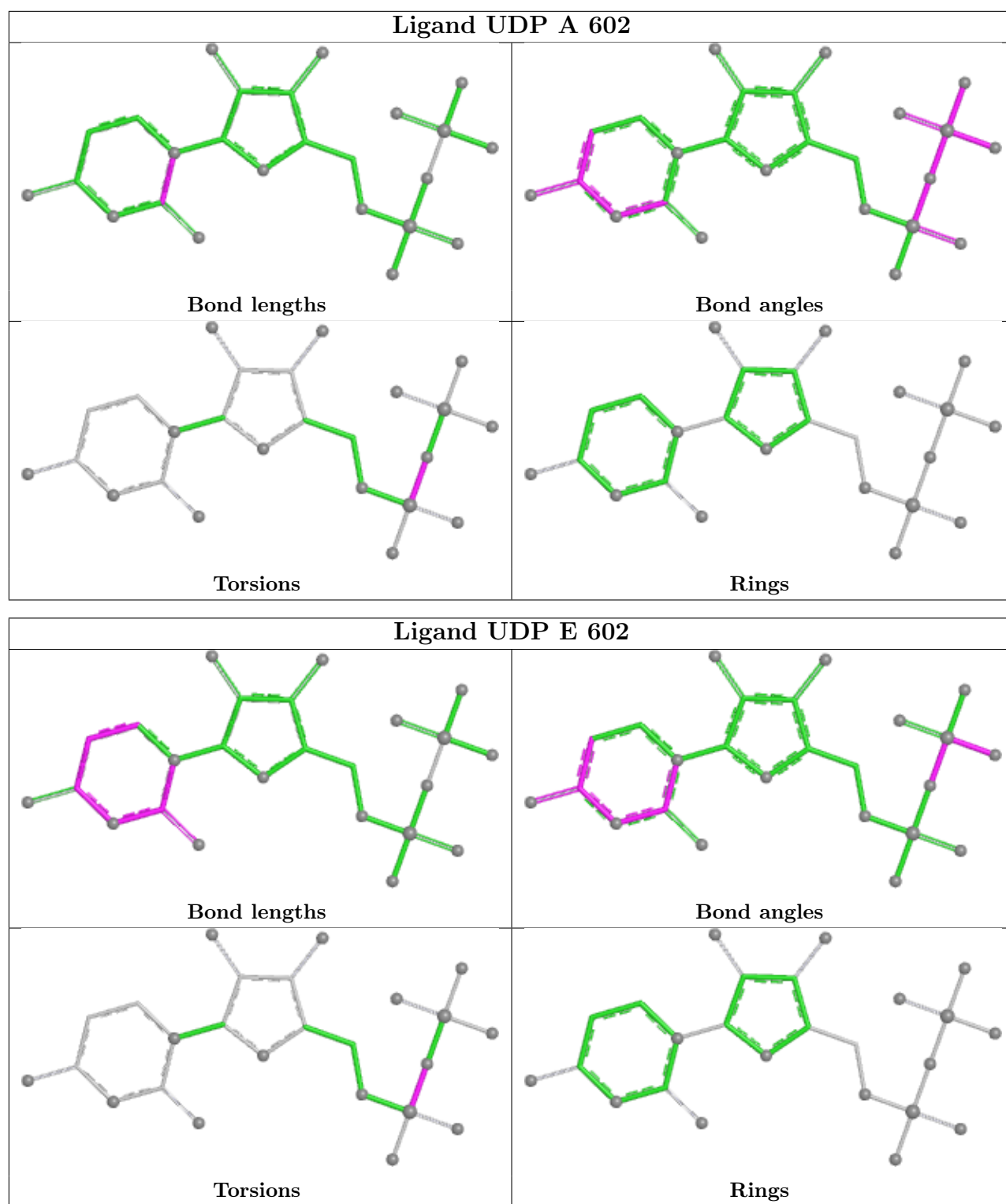


Ligand LU2 A 608



Ligand LU2 B 604





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	495/571 (86%)	-0.20	2 (0%) 88 89	20, 43, 71, 116	7 (1%)
1	B	495/571 (86%)	0.00	6 (1%) 76 77	23, 48, 82, 142	7 (1%)
1	C	495/571 (86%)	0.19	17 (3%) 48 50	25, 51, 87, 172	8 (1%)
1	D	495/571 (86%)	-0.00	9 (1%) 67 69	25, 45, 79, 120	7 (1%)
1	E	492/571 (86%)	0.41	25 (5%) 33 35	27, 61, 106, 176	8 (1%)
1	F	495/571 (86%)	0.37	26 (5%) 32 34	33, 57, 96, 138	6 (1%)
All	All	2967/3426 (86%)	0.13	85 (2%) 53 56	20, 49, 91, 176	43 (1%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	VAL	4.1
1	F	284	TYR	3.7
1	D	377	PHE	3.7
1	C	133	VAL	3.6
1	E	445	ILE	3.6
1	E	88	GLY	3.6
1	F	366	PRO	3.5
1	D	376	VAL	3.5
1	E	447	PHE	3.5
1	E	558	ALA	3.4
1	E	539	CYS	3.4
1	E	559	LEU	3.4
1	B	92	VAL	3.3
1	F	377	PHE	3.3
1	F	371	GLY	3.1
1	E	563	TRP	3.1
1	C	537	ASN	3.0
1	C	557	PRO	3.0
1	F	297	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	90	THR	2.9
1	E	440	PRO	2.9
1	E	531	LEU	2.9
1	F	569	LEU	2.9
1	F	370	PRO	2.9
1	E	484	LEU	2.9
1	C	128	ARG	2.8
1	D	370	PRO	2.8
1	E	552	VAL	2.8
1	F	282	TRP	2.8
1	B	89	GLY	2.7
1	C	92	VAL	2.7
1	E	439	VAL	2.6
1	F	307	ALA	2.6
1	F	369	PHE	2.6
1	E	557	PRO	2.6
1	C	555	CYS	2.6
1	F	290	ARG	2.6
1	E	90	THR	2.6
1	D	409	GLY	2.5
1	C	89	GLY	2.5
1	F	316	PHE	2.5
1	C	556	GLY	2.5
1	F	372	GLY	2.5
1	C	129	LYS	2.5
1	F	330	VAL	2.4
1	D	331	TRP	2.4
1	C	569	LEU	2.4
1	F	133	VAL	2.4
1	F	280	PHE	2.4
1	F	376	VAL	2.4
1	C	283	ASP	2.4
1	E	540	LEU	2.4
1	D	372	GLY	2.3
1	C	538	LEU	2.3
1	C	124	ASP	2.3
1	C	130	GLN	2.3
1	F	96	GLN	2.3
1	F	306	ILE	2.3
1	C	554	VAL	2.3
1	E	565	PHE	2.3
1	F	365	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	367	TYR	2.2
1	D	369	PHE	2.2
1	F	568	ASN	2.2
1	E	476	ALA	2.2
1	B	131	TRP	2.2
1	F	291	ARG	2.2
1	E	534	VAL	2.2
1	E	442	HIS	2.2
1	F	95	GLY	2.2
1	B	569	LEU	2.1
1	C	531	LEU	2.1
1	A	377	PHE	2.1
1	D	463	PHE	2.1
1	F	293	ARG	2.1
1	F	373	SER	2.1
1	E	471	TYR	2.1
1	A	90	THR	2.1
1	C	94	SER	2.1
1	E	456	CYS	2.1
1	E	514	ARG	2.1
1	E	446	ALA	2.0
1	D	411	ILE	2.0
1	E	554	VAL	2.0
1	E	331	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

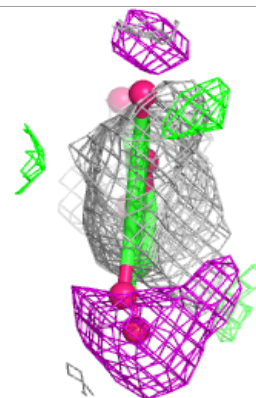
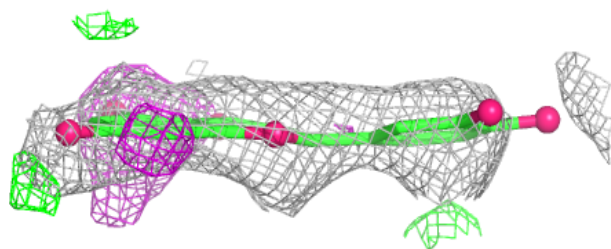
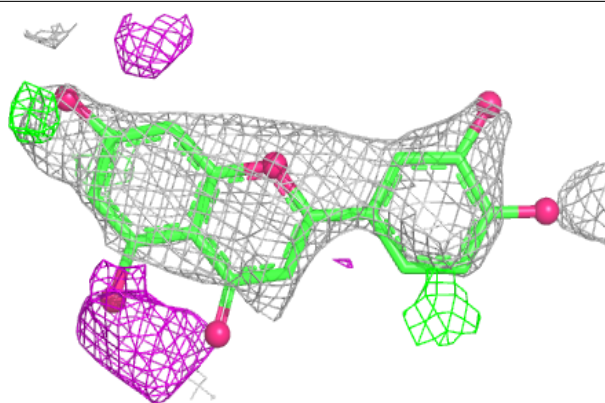
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	C	603	4/4	0.62	0.20	71,79,83,90	0
4	EDO	A	604	4/4	0.71	0.18	44,56,56,57	0
5	LU2	B	604	21/21	0.74	0.21	84,109,128,163	0
5	LU2	D	604	21/21	0.75	0.18	60,107,129,161	0
4	EDO	A	607	4/4	0.77	0.15	79,88,92,96	0
4	EDO	F	603	4/4	0.78	0.17	73,73,73,74	0
4	EDO	E	603	4/4	0.79	0.15	64,68,72,72	0
4	EDO	B	603	4/4	0.81	0.13	54,63,64,65	0
5	LU2	A	608	21/21	0.82	0.17	53,83,117,166	0
4	EDO	A	605	4/4	0.83	0.13	46,49,53,59	0
4	EDO	A	603	4/4	0.84	0.21	51,52,53,53	0
4	EDO	A	606	4/4	0.86	0.11	64,71,74,77	0
4	EDO	D	603	4/4	0.88	0.10	31,33,37,38	0
3	UDP	F	602	25/25	0.93	0.10	53,61,68,71	0
3	UDP	D	602	25/25	0.96	0.07	37,42,49,50	0
3	UDP	E	602	25/25	0.97	0.06	41,49,60,64	0
3	UDP	C	602	25/25	0.97	0.06	38,45,52,55	0
3	UDP	B	602	25/25	0.97	0.06	39,49,64,70	0
3	UDP	A	602	25/25	0.98	0.05	30,39,47,51	0
2	MN	F	601	1/1	0.99	0.02	50,50,50,50	0
2	MN	B	601	1/1	0.99	0.02	43,43,43,43	0
2	MN	C	601	1/1	0.99	0.02	36,36,36,36	0
2	MN	D	601	1/1	0.99	0.02	36,36,36,36	0
2	MN	E	601	1/1	0.99	0.01	40,40,40,40	0
2	MN	A	601	1/1	1.00	0.01	33,33,33,33	0

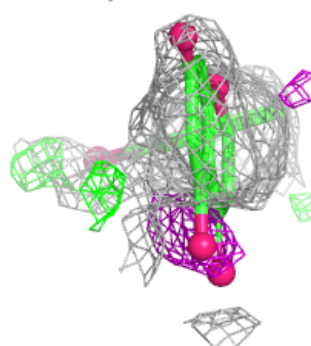
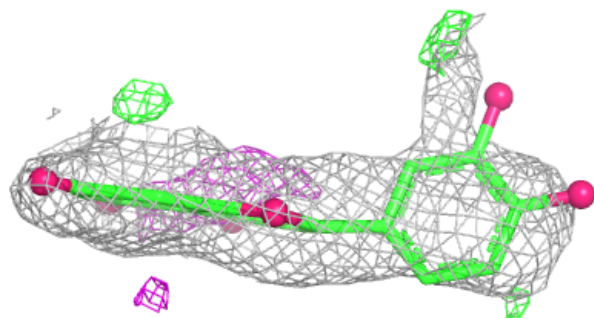
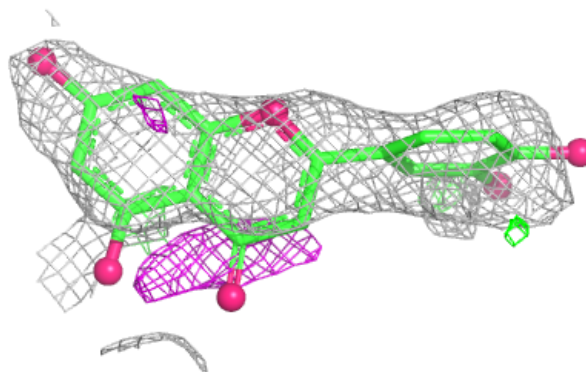
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LU2 B 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

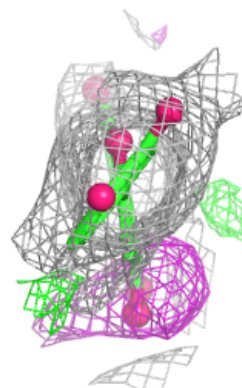
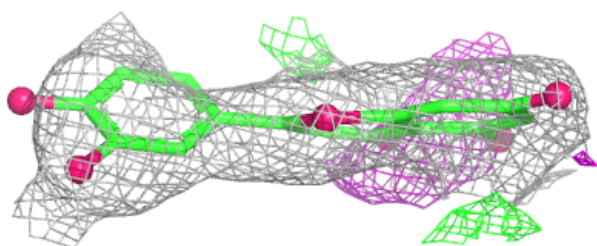
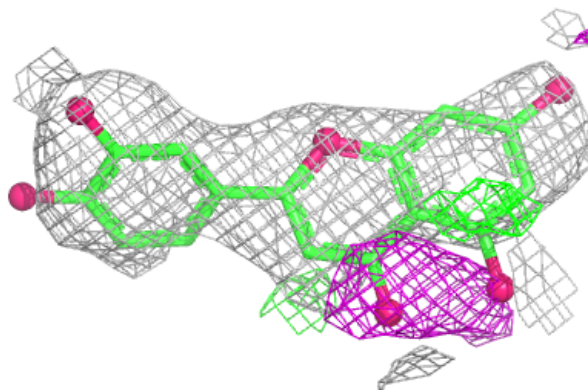
**Electron density around LU2 D 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



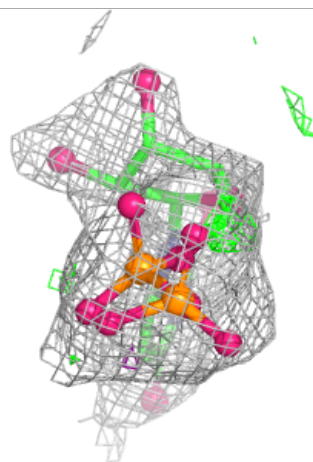
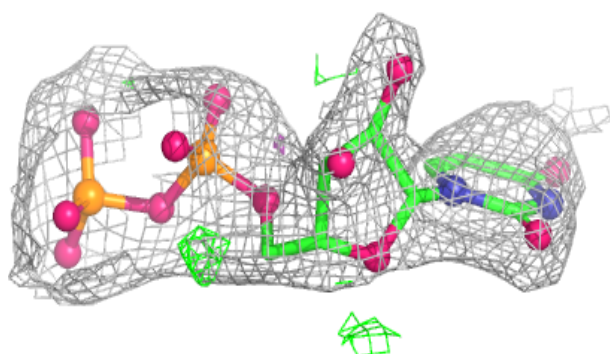
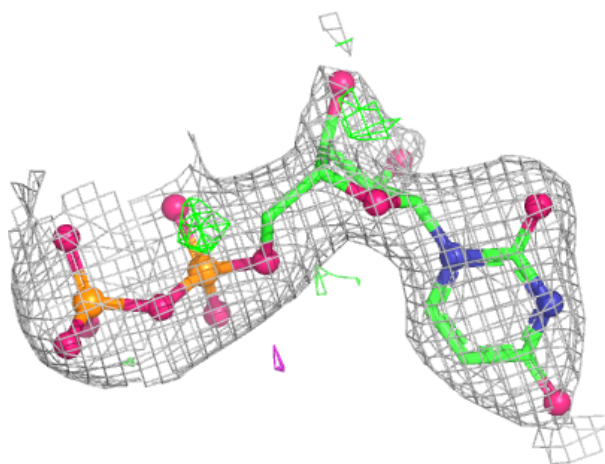
Electron density around LU2 A 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



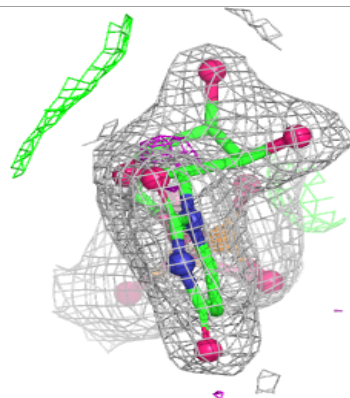
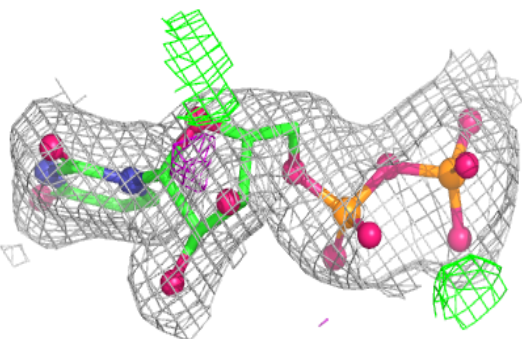
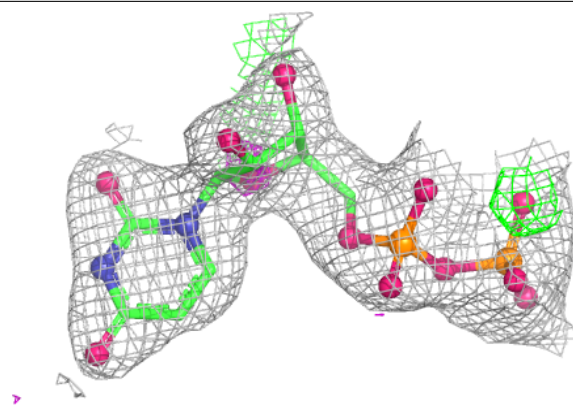
Electron density around UDP F 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

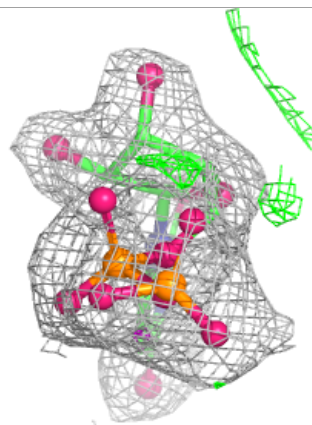
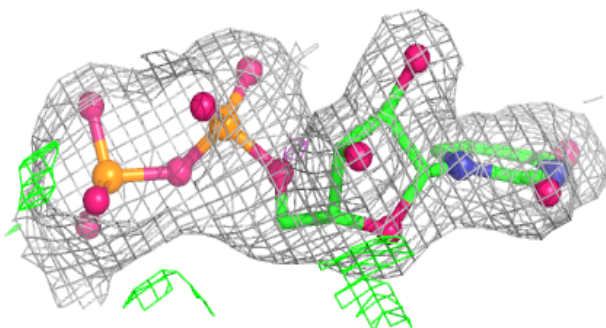
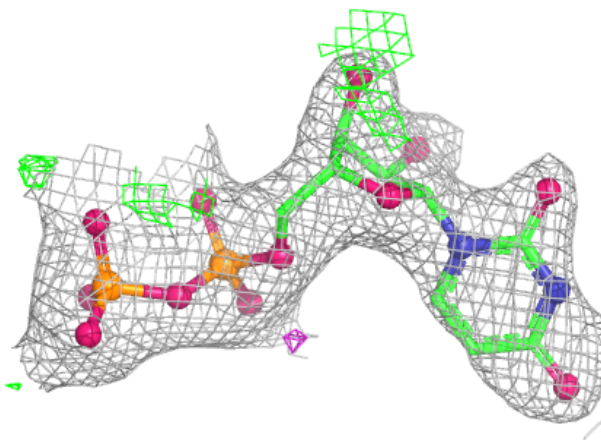


Electron density around UDP D 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

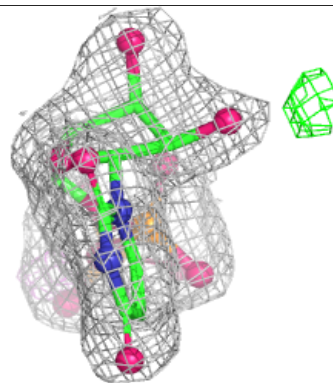
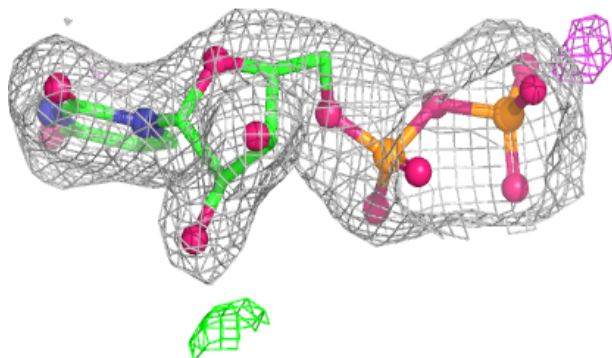
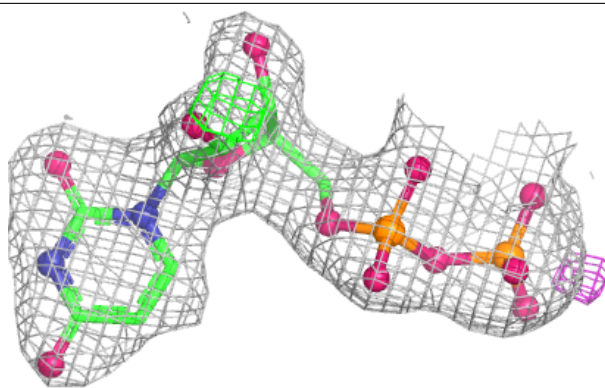
**Electron density around UDP E 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



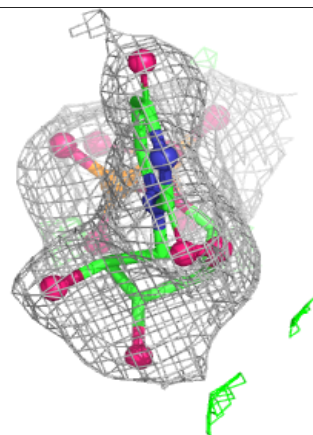
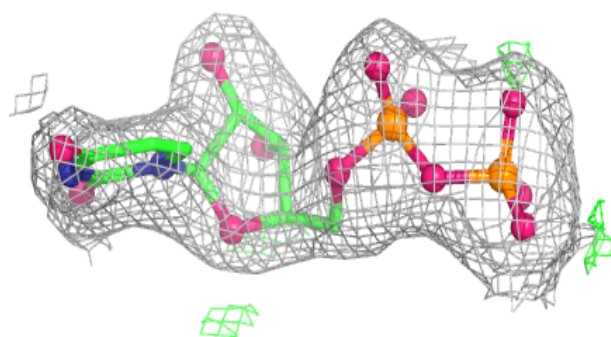
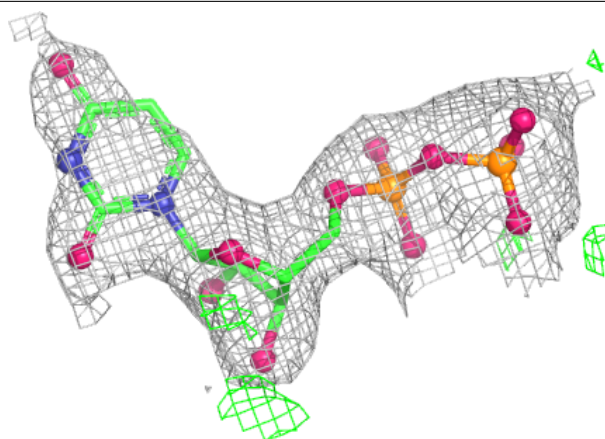
Electron density around UDP C 602:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



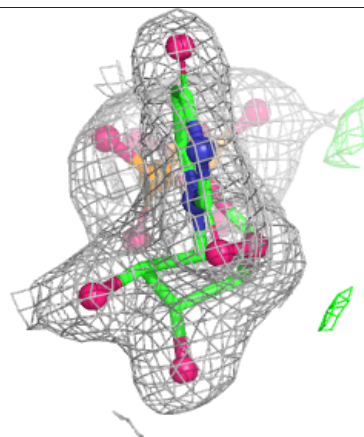
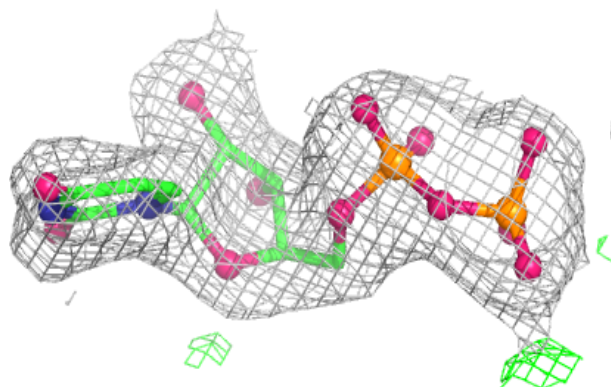
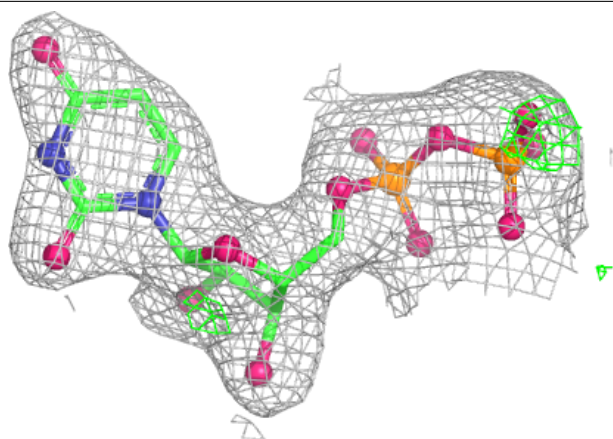
Electron density around UDP B 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UDP A 602:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.